



# ANSYS Chemkin-Pro Input Manual

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# Table of Contents

<b>1. Introduction</b>	1
<b>2. Thermodynamic Data</b>	3
2.1. Thermodynamic Data Format	3
2.1.1. Using More than Two Temperature Ranges	8
2.1.2. Creating Very Large Molecules with Unlimited Number of Elements	8
2.1.3. Surface-Coverage Dependent Enthalpy of Surface Species	9
2.1.4. Gas Species Radiation Absorption Coefficients	9
2.2. Standard State Enthalpies and Entropies at 298 K	11
<b>3. Gas-phase Kinetics Input</b>	33
3.1. Element Data	33
3.2. Species Data	35
3.3. Thermodynamic Data	36
3.4. Real Gas Data	37
3.5. Transport Data	38
3.6. Reaction Mechanism Description	39
3.6.1. REACTIONS Line Options	39
3.6.2. Reaction Data	41
3.6.3. Auxiliary Reaction Data	43
3.6.3.1. Problems Having No Reactions	57
3.6.4. Error Checks	58
<b>4. Surface Kinetics Input</b>	61
4.1. Material Declaration	61
4.2. Site Data	62
4.3. Bulk Data	64
4.4. Thermodynamic Data	65
4.5. Reaction Mechanism Description	66
4.5.1. REACTIONS Line Options	66
4.5.2. Reaction Data	70
4.5.3. Auxiliary Reaction Data	72
4.5.3.1. Summary of Auxiliary Reaction Data	81
4.5.4. Problems Having No Reactions	84
4.5.5. Error Checks	84
<b>5. Transport Database</b>	87
5.1. Transport Data Format	87
5.2. Including Transport Data in the Gas-phase Kinetics Input File	87
5.3. Transport Data Included with CHEMKIN	88
<b>6. Description and Properties of Particles</b>	95
6.1. Description and Properties of the Particle Material	95
6.1.1. Dispersed Material	95
6.1.2. Particle Composition	96
6.1.3. Particle Class	97
6.1.4. Mass and Volume of an Individual Particle	97
6.1.5. Diameter and Surface Area of an Individual Particle	98
<b>7. Using the FITDAT Utility</b>	99
7.1. Running FITDAT from the User Interface	99
7.2. Programming with FITDAT	100
7.3. Keyword Syntax and Rules	101
7.4. FITDAT Keywords	101
7.5. FITDAT Examples	105
7.5.1. DATA CHEM Input Format	105

7.5.2. POLY CHEM Input Format .....	105
7.5.3. DATA NIST Input Format .....	106
7.5.4. POLY SHOM Input Format .....	106
7.5.5. DATA NASA Input Format .....	107
7.5.6. POLY NASA Input Format .....	108
7.5.7. DATA JANAF Input Format .....	108
7.5.8. VIBE Input Format .....	109
7.5.9. Example <i>FITDAT</i> Outputs .....	110
<b>8. CHEMKIN Project Input: Keyword Syntax and Rules .....</b>	<b>113</b>
<b>9. Reference Guide to Project Input Keywords .....</b>	<b>115</b>
9.1. Closed 0-D Reactor Models .....	115
9.1.1. Internal Combustion HCCI Engine .....	115
9.1.2. Closed Homogeneous Batch Reactor .....	115
9.1.3. Closed Partially Stirred Reactor .....	116
9.1.4. Closed Plasma Reactor .....	116
9.1.5. Multi-Zone HCCI Engine Simulator .....	116
9.1.6. SI Engine Zonal Simulator .....	116
9.1.7. Direct Injection Diesel Engine Simulator .....	117
9.2. Open 0-D Reactor Models .....	117
9.2.1. Perfectly Stirred Reactor .....	117
9.2.2. Plasma Perfectly Stirred Reactor .....	117
9.2.3. Partially Stirred Reactor .....	117
9.3. Flow Reactor Models .....	118
9.3.1. Plug Flow Reactor .....	118
9.3.2. Plasma Plug Flow Reactor .....	118
9.3.3. Planar Shear Flow .....	118
9.3.4. Cylindrical Shear Flow .....	119
9.3.5. Honeycomb Monolith Reactor .....	119
9.4. Flame Simulators .....	119
9.4.1. Premixed Laminar Burner-stabilized Flame Simulator .....	119
9.4.2. Flame Speed Simulator .....	120
9.4.3. Opposed-flow Flame Simulator .....	120
9.4.4. Premixed Laminar Burner-stabilized Stagnation Flow Flame Simulator .....	120
9.4.5. Flame-Extinction Simulator .....	120
9.4.6. Diffusion Flamelet Generator .....	121
9.5. CVD Reactors .....	121
9.5.1. Stagnation Flow CVD Reactor .....	121
9.5.2. Rotating Disk CVD Reactor .....	121
9.6. Shock Tube Reactors .....	121
9.6.1. Normal Incident Shock .....	121
9.6.2. Normal Reflected Shock .....	121
9.7. Miscellaneous Reactor Models .....	122
9.7.1. Gas Mixer .....	122
9.7.2. Equilibrium .....	122
9.7.3. Mechanism Analyzer .....	122
<b>10. Alphabetical Listing of Project Input Keywords .....</b>	<b>123</b>
10.1. Alphabetical Listing of Keywords [A-E] .....	123
10.2. Alphabetical Listing of Keywords [F-O] .....	181
10.3. Alphabetical Listing of Keywords [P-S] .....	237
10.4. Alphabetical Listing of Keywords [T-Z] .....	295
Bibliography .....	345

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## List of Figures

2.1. Excerpts from the <i>therm.dat</i> Thermodynamic Database File .....	4
2.2. Examples of Thermodynamic Data .....	7
2.3. Examples of Very Large Molecules .....	8
2.4. HFCOV Thermodynamic Auxiliary Keyword Example .....	9
3.1. Examples of Species Data .....	34
3.2. Examples of Species Data .....	35
3.3. Example of Real Gas data input .....	38
3.4. Examples of Reaction Data .....	42
3.5. Examples of Auxiliary Reaction Data .....	56
4.1. Examples of Material Declarations .....	61
4.2. Examples of Site Data .....	63
4.3. Examples of Bulk Data .....	65
4.4. Examples of Reaction Data .....	71
4.5. Examples of Auxiliary Reaction Data .....	81
6.1. Example of Dispersed Material Declaration .....	95
6.2. Example of Two Material Blocks .....	96
6.3. Dispersed Graphite Material Declaration With Chemical Composition .....	96
6.4. Dispersed Silicon Dioxide Material Declaration With Chemical Composition .....	96
6.5. Nucleation Reaction Creating Particle Nuclei of Class 32 .....	97
7.1. Utilities—'Fitdat' Polynomial Equation Fitter .....	100
7.2. DATA CHEM Input File .....	105
7.3. POLY CHEM Input File .....	105
7.4. DATA NIST Input File .....	106
7.5. POLY SHOM Input File .....	107
7.6. DATA NASA Input File .....	107
7.7. POLY NASA Input File .....	108
7.8. Format details for POLY NASA Input Files .....	108
7.9. DATA JANAF Input File .....	109
7.10. VIBE Input File .....	109
7.11. Example <i>fitdat.out</i> file .....	110
7.12. Example <i>fitdat.out</i> file with more than two temperature ranges .....	110



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## List of Tables

2.1. Summary of the Rules for Thermodynamic Data .....	4
2.2. Fortran Format Descriptions from Table 2.1: Summary of the Rules for Thermodynamic Data .....	6
2.3. Alternative Format for Specifying More than Two Temperature Ranges .....	8
2.4. Standard State Enthalpies and Entropies at 298 K .....	11
3.1. Summary of the Rules for Element Data .....	34
3.2. Summary of the Rules for Species Data .....	36
3.3. Cubic equation of state models available in Chemkin-Pro .....	37
3.4. Alphabetical Listing of REACTIONS-line Options for Gas-phase Kinetics Data .....	39
3.5. Reaction Data Criteria .....	41
3.6. Summary of the Rules for Reaction Data .....	43
3.7. Alphabetical Listing of Gas-phase Reaction Auxiliary Keywords .....	43
3.8. Summary of the Rules for Auxiliary Reaction Data .....	57
3.9. Error Checks .....	58
4.1. Summary of the Rules for Site Data .....	63
4.2. Summary of the Rules for Bulk Data .....	64
4.3. Alphabetical Listing of REACTIONS-line Options for Surface Reaction Data .....	66
4.4. Surface Reaction Data Criteria .....	70
4.5. Summary of the Rules for Reaction Data .....	71
4.6. Alphabetical Listing of Surface Reaction Auxiliary Keywords .....	72
4.7. Summary of the Rules for Auxiliary Reaction Data .....	82
4.8. Error Checks .....	84
5.1. Species in <i>Transport</i> Database .....	88
7.1. Summary of Rules for Keywords .....	101
7.2. <i>FITDAT</i> Keywords .....	101
8.1. Summary of the Rules for Keywords .....	113
10.1. Alphabetical Listing of Keywords [A-E] .....	123
10.2. Alphabetical Listing of Keywords [F-O] .....	181
10.3. Alphabetical Listing of Keywords [P-S] .....	237
10.4. Alphabetical Listing of Keywords [T-Z] .....	295





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## Chapter 1: Introduction

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The [Chemkin-Pro Input Manual \(p. 1\)](#) is designed to serve as a reference to ANSYS Chemkin-Pro users who require more information about the input parameters needed in defining a chemically reacting flow simulation. In particular, information about syntax and format of chemical reaction mechanism input files, thermodynamic data, and transport-property data are described in detail. In addition, detailed information about all of the input parameters associated with reactor models, including default values and usage guidelines, are included in the Keywords section.

The ANSYS Chemkin-Pro Interface guides users through problem setup and execution, as well as quick analysis with the Chemkin-Pro Visualizer. The operation of the Chemkin-Pro Interface and Post-Processing are described in detail in [Chemkin-Pro Getting Started Guide](#). In some cases, however, users may wish to work from the command line instead of the User Interface and manually assemble Reactor Model input files. For this purpose, the [Chemkin-Pro Input Manual \(p. 1\)](#) describes the necessary syntax and usage of the reactor-input Keywords, as well as a quick reference of what keywords are available for each Reactor Model.

For background information on the equations and theory behind the input parameters, the [Chemkin-Pro Theory Manual](#) provides further reading. In many cases, equations in the [Chemkin-Pro Theory Manual](#) are references in the discussions of reactor parameter input Keywords.

In [Thermodynamic Data \(p. 3\)](#) through [Transport Database \(p. 87\)](#), we describe the syntax and format required for thermodynamic, gas-phase kinetics, surface kinetics, and transport-property input data. [Description and Properties of Particles \(p. 95\)](#) has the description of fundamental particle properties for Particle Tracking. [CHEMKIN Project Input: Keyword Syntax and Rules \(p. 113\)](#) provides an overview of the syntax and rules for Keyword input, which make up the Reactor Model input files. Reactor Model input files are ordinarily created by the User Interface but can also be manually assembled for command-line usage. [Reference Guide to Project Input Keywords \(p. 115\)](#) provides a Quick Reference of the Keywords, organized by Reactor Model and other concepts, while [Alphabetical Listing of Project Input Keywords \(p. 123\)](#) contains alphabetical listings of keywords.



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## Chapter 2: Thermodynamic Data

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Any chemical species that appears in a problem must have thermodynamic data associated with it. The format required for these data is described in this chapter. Also [Standard State Enthalpies and Entropies at 298 K \(p. 11\)](#) includes a discussion and listing of the standard-state enthalpies and entropies for the data contained in the therm.dat database file, which is included with every ANSYS Chemkin-Pro installation.

Thermodynamic data may be extracted from a database file (for example, *therm.dat*) and/or read from the *Gas-phase Kinetics* or *Surface Kinetics* input file. If all of the thermodynamic data are to be extracted from a database file, then no thermodynamic data input in the *Gas-phase Kinetics* or *Surface Kinetics* input file is required. However, if the user wishes to override information in the database or to provide data on species not in the database, then thermodynamic data are needed in the *Gas-phase Kinetics* or *Surface Kinetics* input file. In any case, the format for the information is the same.

### 2.1. Thermodynamic Data Format

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ANSYS Chemkin-Pro expects the thermodynamic data to be provided in a specific format. In addition to the fourteen polynomial fitting coefficients (described in [Standard-state Thermodynamic Properties in the Chemkin-Pro Theory Manual](#)), the database also contains the species' name, its elemental composition, its electronic charge, and an indication of its phase (gas, liquid or solid). The data for each species requires four formatted lines of length 80 characters. [Figure 2.1: Excerpts from the therm.dat Thermodynamic Database File \(p. 4\)](#) is a sample of the lines required for a species and [Table 2.1: Summary of the Rules for Thermodynamic Data \(p. 4\)](#) provides a detailed specification of the format required for entry of thermodynamics data. The first two lines in [Figure 2.1: Excerpts from the therm.dat Thermodynamic Database File \(p. 4\)](#) are required at the top of a thermodynamic database file; the first line specifies that the following is a set of thermodynamic data, while the second line provides the three temperatures used in the fitting process (a low temperature, break temperature, and high temperature). The user must also adhere to these specifications when placing thermodynamic data within the *Gas-phase Kinetics* or *Surface Kinetics* input file.

The default format (see [Table 2.1: Summary of the Rules for Thermodynamic Data \(p. 4\)](#) and [Table 2.2: Fortran Format Descriptions from Table 2.1: Summary of the Rules for Thermodynamic Data \(p. 6\)](#)) is a minor modification of that used by Gordon and McBride[1] (p. 345) for the Thermodynamic Database in the NASA Chemical Equilibrium code. However, ANSYS Chemkin-Pro allows a different midpoint temperature for the fits to the properties of each chemical species. We also allow a species to be composed of a maximum of nine elements, not four, on Line 3. Additional extensions allowed by Chemkin-Pro for multiple temperature ranges and for very large molecular clusters are described in [Using More than Two Temperature Ranges \(p. 8\)](#) and [Creating Very Large Molecules with Unlimited Number of Elements \(p. 8\)](#), respectively. Despite these extensions, however, Chemkin-Pro can use the NASA database directly without any modification. The format conventions are summarized in [Table 2.2: Fortran Format Descriptions from Table 2.1: Summary of the Rules for Thermodynamic Data \(p. 6\)](#).

As indicated in [Table 2.1: Summary of the Rules for Thermodynamic Data \(p. 4\)](#), the pertinent information includes the species name, the elemental composition of the species, and the temperature ranges

over which the polynomial fits to thermodynamic data are valid. The fits to  $C_p^o/R$ ,  $H^o/RT$ , and  $S^o/R$  consist of seven coefficients for each of two temperature ranges, see [Equation 2.18](#), [Equation 2.22](#) and [Equation 2.28](#) of the [Chemkin-Pro Theory Manual](#). Further information about the fitting procedure can be found in the [Chemkin-Pro Theory Manual](#) as well as [Using the FITDAT Utility \(p. 99\)](#).

### Note:

Some users enhance the Thermodynamic Data block with additional data, such as tags for liquid fuel properties, SMILES, etc. These property tags are described in [Format for Property Tagging in the Chemkin-Pro Reaction Workbench User's Manual](#). The supplemental data are used by several ANSYS Chemkin-Pro features, including the Reaction Path Analyzer (see the [Chemkin-Pro Visualization Manual](#)) and the Surrogate Blend Optimizer (see the [Chemkin-Pro Reaction Workbench User's Manual](#)).

**Figure 2.1: Excerpts from the *therm.dat* Thermodynamic Database File**

```

THERMO
  300.000  1000.000  5000.000
(CH2O)3      70590C  3H  6O  3      G  0300.00  4000.00  1500.00      1
  0.01913678E+03  0.08578044E-01-0.08882060E-05-0.03574819E-08  0.06605142E-12      2
-0.06560876E+06-0.08432507E+03-0.04662286E+02  0.06091547E+00-0.04710536E-03      3
  0.01968843E-06-0.03563271E-10-0.05665403E+06  0.04525264E+03      4
AL      62987AL  1      G  0300.00  5000.00  0600.00      1
  0.02559589E+02-0.10632239E-03  0.07202828E-06-0.02121105E-09  0.02289429E-13      2
  0.03890214E+06  0.05234522E+02  0.02736825E+02-0.05912374E-02-0.04033937E-05      3
  0.02322343E-07-0.01705599E-10  0.03886794E+06  0.04363879E+02      4
END

```

**Table 2.1: Summary of the Rules for Thermodynamic Data**

Line #	Contents	Format <sup>a</sup>	Note in following table <sup>b</sup>	Column
1	THERMO (or THERMO ALL) <sup>c</sup>	Free	c	Any
2	Temperature ranges for 2 sets of coefficients: lowest T, common T, and highest T <sup>d</sup>	3F10.0	d	1 to 30
3	Species name (must start in Column 1)	16A1	e	1 to 16
	Date (not used)	6A1	f	19 to 24
	Atomic symbols and formula	4(2A1, I3)	g	25 to 44
	Phase of species (S, L, or G for solid, liquid, or gas)	A1	h	45
	Low temperature	E10.0	i	46 to 55

Line #	Contents	Format <sup>a</sup>	Note in following table <sup>b</sup>	Column
	High temperature	E10.0	i	56 to 65
	Common temperature (if needed, else blank)	E8.0	j	66 to 73
	Atomic symbols and formula (if needed, else blank)	2A1, I3	k	74 to 78
	The integer 1. This is a <b>mandatory</b> element and <b>must</b> appear in column 80.	I1	l	80
	Atomic symbols and formula (if needed, else blank), or & to indicate continuation to next line (See <a href="#">Creating Very Large Molecules with Unlimited Number of Elements</a> (p. 8) for further information)	4(2A1, I3)	g	81 to 100
4	Coefficients $a_1$ through $a_5$ in <a href="#">Equation 2.18</a> , <a href="#">Equation 2.22</a> and <a href="#">Equation 2.28</a> of the <a href="#">Chemkin-Pro Theory Manual</a> , for upper temperature interval	5(E15.8)	m	1 to 75
	The integer 2	I1	l	80
5	Coefficients $a_6$ , $a_7$ for upper temperature interval, and $a_1$ , $a_2$ , and $a_3$ for lower temperature interval	5(E15.8)	m	1 to 75
	The integer 3	I	l	80
6	Coefficients $a_4$ , $a_5$ , $a_6$ , $a_7$ for lower temperature interval	4(E15.8)	n	1 to 60
	The integer 4	I1	l	80
..	Repeat lines 3 - 6 for each species			
last	End (Optional, end of thermodynamic data.)	Free	c	Any

<sup>a</sup>The format string in this column follows the convention of FORTRAN documentation, as detailed in the notes provided in [Table 2.2: Fortran Format Descriptions](#) from [Table 2.1: Summary of the Rules for Thermodynamic Data](#) (p. 6).

<sup>b</sup>See [Table 2.2: Fortran Format Descriptions](#) from [Table 2.1: Summary of the Rules for Thermodynamic Data](#) (p. 6)

<sup>c</sup>Use only when all thermodynamic data are to be taken from Pre-processor input.

<sup>d</sup> When inserting thermodynamic data directly in the *Gas-phase Kinetics* and *Surface Kinetics* input files, Line 2 should only be included with THERMO ALL option (See *Gas-phase Kinetics* and *Surface Kinetics* for more information).

**Table 2.2: Fortran Format Descriptions from Table 2.1: Summary of the Rules for Thermodynamic Data (p. 4)**

Note	Format	Format Description
c	FREE	The particular input described can be in any column of the input line.
d	3F10.0	3 Floating-point (real) values are allowed; each is allocated 10 columns.
e	16A1	16 Alpha-numeric characters are allowed in these columns (some may be blank).
f	6A1	6 Alpha-numeric characters are allowed in these columns (some may be blank).
g	4(2A1,I3)	There can be 4 sets of data; each set is allowed 2 Alpha-numeric columns (an element symbol) followed by 3 columns containing an Integer value (element count).
h	A1	1 Alpha-numeric character is allowed.
i	E10.0	10 columns are allocated for a real value, and scientific notation (E format) is allowed.
j	E8.0	8 columns are allocated for a real value, and scientific notation (E format) is allowed.
k	2A1,I3	2 Alpha-numeric columns (an element symbol) followed by 3 columns for an integer value (element count).
l	I1	One column is allowed for an integer value.
m	5(E15.8)	5 real values are allowed, with 15 columns allocated for each value, and scientific notation is allowed to have up to 8 values after the decimal point.
n	4(E15.8)	4 real values are allowed, with 15 columns allocated for each value, and scientific notation is allowed to have up to 8 values after the decimal point.

The first thermodynamic data line must start with the word THERMO (or THER). If the data appears inside of a *Gas-phase Kinetics* or *Surface Kinetics* input file, then the addition entry ALL (i.e., the first line reads THERMO ALL) tells the pre-processor that all thermodynamic data for the species associated with that chemistry input are included in the chemistry input file. This will cause the pre-processor not to try to open or read a Thermodynamic database file.

If the data are in a thermodynamics database file, or if THERMO ALL precedes within a *Gas-phase Kinetics* or *Surface Kinetics* input file, then the next line must be Line 2 of Table 2.1: Summary of the Rules for Thermodynamic Data (p. 4). Otherwise Line 2 is skipped. In any case, the subsequent thermodynamic data lines must be in the format of Lines 3 - 6 of Table 2.1: Summary of the Rules for Thermodynamic Data (p. 4). (For the THERMO option within a kinetics input file, the midpoint temperature is taken from Line 2 information already in the Thermodynamic Database associated with the chemistry set.)

Figure 2.2: Examples of Thermodynamic Data (p. 7) shows some examples of thermodynamic property input, as they might occur within a *Gas-phase Kinetics* input file. In these examples for OH, OH<sup>+</sup>, and OH<sup>-</sup>, it is seen from columns 25 - 34 that the elemental composition of each molecule is one O atom

and one H atom. In addition, columns 35 - 39 indicate that two of the species, OH<sup>+</sup>, and OH<sup>-</sup>, are ionic since they contain -1 and +1 electrons (E), respectively. The G in column 45 indicates that all three species are gaseous. (This phase information is ignored by *Gas-phase Kinetics*.) The 1000.00 in columns 66 - 73 for OH indicates that the common temperature between the high- and low-temperature fits is 1000.00 K. If columns 66 - 73 are left blank, as they are for OH<sup>+</sup> and OH<sup>-</sup>, then the common temperature is that given in columns 11 - 20 in [Table 2.1: Summary of the Rules for Thermodynamic Data \(p. 4\)](#), which in this example is in the Thermodynamic Database. An alternative format is shown for OH if more than two temperature ranges are required. In this case we've given the molecule a different name, "MyOH", but the elemental composition is the same as for OH. The line after the elemental composition contains the TEMP description of minimum, common, and maximum temperatures, and a set of coefficients for each temperature range, ordered from highest to lowest.

**Figure 2.2: Examples of Thermodynamic Data**

```

THERMO
OH          1212860  1H  1      G  0300.00  5000.00  1000.00      1
0.02882730E+02 0.10139743E-02-0.02276877E-05 0.02174683E-09-0.05126305E-14 2
0.03886888E+05 0.05595712E+02 0.03637266E+02 0.01850910E-02-0.16761646E-05 3
0.02387202E-07-0.08431442E-11 0.03606781E+05 0.13588605E+01 4
OH+         1212860  1H  1E -1  G  0300.00  5000.00      1
0.02719058E+02 0.15085714E-02-0.05029369E-05 0.08261951E-09-0.04947452E-13 2
0.15763414E+06 0.06234536E+02 0.03326978E+02 0.13457859E-02-0.03777167E-04 3
0.04687749E-07-0.01780982E-10 0.15740294E+06 0.02744042E+02 4
OH-         1212860  1H  1E  1  G  0300.00  5000.00      1
0.02846204E+02 0.10418347E-02-0.02416850E-05 0.02483215E-09-0.07775605E-14 2
-0.01807280E+06 0.04422712E+02 0.03390037E+02 0.07922381E-02-0.01943429E-04 3
0.02001769E-07-0.05702087E-11-0.01830493E+06 0.12498923E+01 4
MyOH        00  1H  1  0  0G  300.000  5000.000      0 1
TEMP  300.000  1000.000  2500.000  5000.000
0.30563941E+01 0.89059362E-03-0.20849917E-06 0.24115927E-10-0.10516720E-14
0.37260112E+04 0.44780081E+01
0.34298433E+01-0.25250392E-03 0.80470663E-06-0.33336490E-09 0.43425671E-13
0.37097800E+04 0.26751302E+01
0.37695923E+01-0.59256858E-03-0.21359336E-06 0.13644331E-08-0.63575666E-12
0.35908836E+04 0.78130486E+00
END

```

The following is a summary of the possibilities for specifying thermodynamic data:

- **Case 1:** All thermodynamic data from database file
  1. A database file is opened during pre-processing (e.g. *therm.dat*).
  2. No THERMO data required in the *Gas-phase* or *Surface Kinetics* input file.
- **Case 2:** Thermodynamic data from database and input files
  1. A database file is opened during pre-processing (e.g. *therm.dat*).
  2. Include the following lines in the *Gas-phase* or *Surface Kinetics* input file, after the species data:

```

THERMO
Data in Table 2.1: Summary of the Rules for Thermodynamic Data \(p. 4\)
format (lines 3 - 6 repeated) for each species not in the database or to override species in database
END

```

- **Case 3:** All thermodynamic data from input file
  1. No Thermodynamic database file is required.

2. Include the following lines in the *Gas-phase* or *Surface Kinetics* input file, after the species data:

```
THERMO ALL
Data in Table 2.1: Summary of the Rules for Thermodynamic Data (p. 4)

format (lines 3 - 6 repeated) for at least all species named in the species data
END
```

### 2.1.1. Using More than Two Temperature Ranges

An alternative input data format allows specification of more than two temperature ranges. Use of this format provides more flexibility in describing the thermodynamic data for complex functions of temperature. This alternative approach is summarized in [Table 2.3: Alternative Format for Specifying More than Two Temperature Ranges \(p. 8\)](#). The alternative lines used in place of lines 4 - 6 of [Table 2.1: Summary of the Rules for Thermodynamic Data \(p. 4\)](#). Line 1 specifies all of the temperature values that define the temperature intervals. Lines 2 and Line 3 are then repeated for each specified temperature interval, in descending order of temperature ranges.

**Table 2.3: Alternative Format for Specifying More than Two Temperature Ranges**

Alternative lines for more than 2 temperature intervals (in place of Lines 4 - 6 in <a href="#">Table 2.1: Summary of the Rules for Thermodynamic Data (p. 4)</a> ):			
Line #	Contents	Format	Column
1	TEMP followed by space-delimited minimum fit temperature, common temperatures in increasing order, and maximum fit temperature.	A4, Free	1 to 80
2	Coefficients $a_1 - a_5$ for a temperature interval	5(E15.8)	1 to 75
3	Coefficients $a_6, a_7$ for a temperature interval	2(E15.8)	1 to 30

### 2.1.2. Creating Very Large Molecules with Unlimited Number of Elements

There are some cases where users may want to define very large molecules that contain many elements or that may be composed of a very large number of atoms for a particular element. For this purpose, we have extended the thermodynamic data format to allow users to provide an unlimited number of elements and unconstrained composition. [Figure 2.3: Examples of Very Large Molecules \(p. 8\)](#) shows an example (for illustration purposes only) of using this extended format to describe a molecule called CLUSTER1 that consists of 2326 carbon atoms, 895 hydrogen atoms, 18 nitrogen atoms, 53 oxygen atoms, and 32 sulfur atoms. The extended format is enabled by putting a & character at the end of Line 3 ([Table 2.1: Summary of the Rules for Thermodynamic Data \(p. 4\)](#)), in column 81. Any number of continuation lines may subsequently be included by adding an ampersand (&) at the end of a preceding line. The composition information used on these continuation lines is in free format, which consists of an element symbol, followed by the number of those atoms in the molecule, followed by another element symbol, and so forth.

**Figure 2.3: Examples of Very Large Molecules**

```
CLUSTER1      121086      G   300.000  5000.000 1000.00      1&
C 2326 H 895 N 18 O 53 S 32
```



```

2.60208700e+00-1.78708100e-04 9.08704100e-08-1.14993300e-11 3.31084400e-16 2
8.54215400e+04 4.19517700e+00 2.49858500e+00 8.08577700e-05-2.69769700e-07 3
3.04072900e-10-1.10665200e-13 8.54587800e+04 4.75345900e+00 4

```

### 2.1.3. Surface-Coverage Dependent Enthalpy of Surface Species

The enthalpy of surface species can be specified to be dependent on surface coverage by entering a block of data starting with `HFCOV` within a block of thermodynamics data that is being specified for surface species. Coverage-dependent coefficients are a subset of the thermodynamic data, and are specified at the end of the surface thermodynamic data input. The linear coverage-dependent coefficients are explicitly specified under the `HFCOV` block, as shown below. The required input for each line consists of the species (*species\_name*) whose enthalpy is dependent on the second mentioned species coverage (*species\_name*), and the coverage-dependent coefficient. The coverage-dependent coefficients must be specified in units of Kelvin.

*Species\_name*<sub>j</sub> *Species\_name*<sub>m</sub> *c*<sub>j,m</sub>

**Figure 2.4: HFCOV Thermodynamic Auxiliary Keyword Example**

```

THERMO
O(S)          C   OH   OO   1AG 1S  0300.00  5000.00  1000.00  1
0.02542059E+02-0.02755061E-03-0.03102803E-07 0.04551067E-10-0.04368051E-14 2
0.02923080E+06 0.04920308E+02 0.02946428E+02-0.16381665E+02 0.02421031E-04 3
-0.16028431E-08 0.03890696E-11 0.02914764E+06 0.02963995E+02 4
C2H4(S)       C   2H   4O   0AG 1S  0298.00  5998.00  1298.00  1
0.68302018E+01 0.10144574E-01-0.34419787E-05 0.52897660E-09-0.30353490E-13 2
-0.98191467E+04-0.14816284E+02-0.40212793E+00 0.23298220E-01-0.80872187E-05 3
-0.25065598E-08 0.15984527E-11-0.71721868E+04 0.24925868E+02 4
Cl(S)         C   OH   OCl  1AG 1S  0298.00  5998.00  1298.00  1
0.68302018E+01 0.10144574E-01-0.34419787E-05 0.52897660E-09-0.30353490E-13 2
-0.98191467E+04-0.14816284E+02-0.40212793E+00 0.23298220E-01-0.80872187E-05 3
-0.25065598E-08 0.15984527E-11-0.71721868E+04 0.24925868E+02 4

HFCOV ! UNITS ARE KELVIN (ENTHALPY UNITS/GAS CONSTANT)

O(S) O(S)      17966.784

O(S) C2H4(S)   -1811.777

O(S) Cl(S)     1409.160

C2H4(S) Cl(S)  -4932.058

END

END

```

### 2.1.4. Gas Species Radiation Absorption Coefficients

For a gas species to absorb or emit infrared energy, its molecular structure must allow rotational and vibrational transitions and change in dipole moment. Accordingly, all monatomic species, such as O and H, and homonuclear diatomic species, such as O<sub>2</sub>, H<sub>2</sub>, and N<sub>2</sub>, are “transparent” with respect to thermal radiation transfer. Most species that are actively absorbing and emitting infrared energy in flames can be neglected in the radiation calculation because they either have very low concentrations (e.g., NO and NO<sub>2</sub>) or exist in cooler regions of the flow domain (e.g., hydrocarbon fuel species and CH<sub>3</sub> OH). The most important radiating species in hydrocarbon flames are CO<sub>2</sub> and H<sub>2</sub> O. The next

important gas species are CO and CH<sub>4</sub>, which emit about 1/10 as much infrared energy as the two dominant species.

The Planck mean absorption coefficients  $a$  for CO<sub>2</sub>, H<sub>2</sub>O, CO, and CH<sub>4</sub> can be calculated by a narrow-band absorption coefficient model such as RADCAL.[2] (p. 345) Since narrow-band calculations require integrating absorption-line intensities over all wavelengths, direct integration of a narrow-band model into the radiation model would greatly decrease the computational performance. In order to incorporate good absorption coefficient data without sacrificing performance, we instead use polynomials to fit to temperature to represent the absorption coefficient data for individual gas species.[3] (p. 345)

Two types of temperature polynomials are accepted by the radiation model for gas species:

- **Polynomial 1:**

$$a_i(T) = \sum_j c_j T^j \quad \text{with } j=0, \dots, 6. \quad (\text{m}^{-1}\text{atm}^{-1}) \quad (2.1)$$

- **Polynomial 2:**

$$a_i(T) = \sum_j c_j / T^j \quad \text{with } j=0, \dots, 6. \quad (\text{m}^{-1}\text{atm}^{-1}) \quad (2.2)$$

The curve-fitting parameters  $c_j$  are entered as optional-data lines in the thermodynamic data file or in the thermodynamic data section of the mechanism input file. The absorption coefficient data line is formatted as

```
![_ AbsorptionCoefficient=" polynomial_form Tmin Tmax c0 c1 c2 c3 c4 c5 c6 " _]
```

AbsorptionCoefficient is the tag indicating the data are for species absorption coefficient calculation. polynomial\_form indicates the form of polynomial used to fit the absorption coefficient. This must have a value of 1.0 or 2.0, corresponding to Equation 2.1 (p. 10) or Equation 2.2 (p. 10), respectively. Tmin is the lower temperature bound in [K] for the fitted curve to be valid. Tmax is the upper temperature bound in [K] for the fitted curve to be valid.  $c_j$  are the seven parameters of the polynomial.

This data line must appear before the thermodynamic data of the associated gas species. Different gas species can use a different form of polynomial. Each gas species can have as many as two absorption-coefficient data lines, which allows two sets of parameters of different temperature ranges. If there are two tag lines for a given gas species, they must be of the same type of polynomial and the low-temperature line should appear before the high-temperature line. The gas radiation model will not be activated if no absorption-coefficient data are included in the thermodynamic data file.

For example, the absorption coefficient data of CO are fitted to two type-1 polynomials over temperature ranges of 300—750 K and 750—2500 K, with the coefficients included in the optional-data lines as follows:

```
![_ AbsorptionCoefficients=" 1 300 750 4.8E0 -6.95E-2 2.96E-4 -4.26E-7 2.03E-10 0 0 " _]
![_ AbsorptionCoefficients=" 1 750 2500 10. -1.2E-2 4.78E-6 -5.87E-10 -2.53E-14 0 0 " _]
CO TPIS79C 10 1 00 00G 200.000 3500.000 1000.000 1
2.71518561E+00 2.06252743E-03 -9.98825771E-07 2.30053008E-10 -2.03647716E-14 2
-1.41518724E+04 7.81868772E+00 3.57953347E+00 -6.10353680E-04 1.01681433E-06 3
9.07005884E-10 -9.04424499E-13 -1.43440860E+04 3.50840928E+00 8.67100000E+03 4
```

## 2.2. Standard State Enthalpies and Entropies at 298 K

Table 2.4: Standard State Enthalpies and Entropies at 298 K (p. 11) contains the standard state enthalpies and entropies for 778 species that are in the thermodynamic database file, *therm.dat* (see Figure 2.1: Excerpts from the *therm.dat* Thermodynamic Database File (p. 4) and Table 2.1: Summary of the Rules for Thermodynamic Data (p. 4) for the data and formats), which is included with all ANSYS Chemkin-Pro installs. The values in the table were determined by evaluating the polynomial expressions (Equation 2.3 (p. 11) and Equation 2.4 (p. 11) of the Chemkin-Pro Theory Manual ) at the standard temperature of 298 K. Note the measured or derived data for  $H^o(298)$  and  $S^o(298)$  that were used in generating the coefficients in *therm.dat* are also included in Table 2.4: Standard State Enthalpies and Entropies at 298 K (p. 11) for comparison.

$$H^o(298) = RT \left[ a_1 + \frac{a_2}{2} T + \frac{a_3}{3} T^2 + \frac{a_4}{4} T^3 + \frac{a_5}{5} T^4 + \frac{a_6}{T} \right] \quad (2.3)$$

$$S^o(298) = R \left[ a_1 \ln T + a_2 T + \frac{a_3}{2} T^2 + \frac{a_4}{3} T^3 + \frac{a_5}{4} T^4 + a_7 \right] \quad (2.4)$$

The units for enthalpies are (kcal)/mole and for entropies cal/(mole · K). The entries in Table 2.4: Standard State Enthalpies and Entropies at 298 K (p. 11) correspond to the *therm.dat* distributed with ANSYS Chemkin-Pro.

**Table 2.4: Standard State Enthalpies and Entropies at 298 K**

Species	$H^o(298)$ kcal/mole		$S^o(298)$ cal/(mole·K)	
	Data	Fit	Data	Fit
(CH <sub>2</sub> O) <sub>3</sub>	-110.70	-110.71	69.42	69.38
(CH <sub>3</sub> ) <sub>2</sub> SiCH <sub>2</sub>	12.30	12.37	80.37	82.41
AL	78.80	78.80	39.30	39.30
AL <sub>2</sub> H <sub>6</sub>	21.35	21.35	62.75	62.75
AL <sub>2</sub> ME <sub>6</sub>	-61.20	-61.20	131.05	131.06
ALAS	107.33	107.32	60.65	60.65
ALH	62.00	62.00	44.88	44.87
ALH <sub>2</sub>	41.95	41.95	54.40	54.40
ALH <sub>3</sub>	18.83	18.83	52.30	52.30
ALME	19.75	19.75	60.68	60.68
ALME <sub>2</sub>	12.75	12.75	77.40	77.40
ALME <sub>3</sub>	-20.30	-20.30	83.68	83.68
AR	0.00	0.00	36.98	36.98
AR+	364.91	364.91	39.75	39.74
AS	75.48	75.48	43.53	43.52
AS <sub>2</sub>	47.08	47.08	59.83	59.83
AS <sub>3</sub>	65.35	65.35	77.53	77.53
AS <sub>4</sub>	37.13	37.13	78.45	78.45
ASALME	70.00	70.00	81.60	81.60
ASALME <sub>2</sub>	63.25	63.25	91.00	91.00
ASGAET	82.75	82.75	95.20	95.20

Species	$H^o(298)\text{kcal/mole}$		$S^o(298)\text{cal/(mole}\cdot\text{K)}$	
	Data	Fit	Data	Fit
ASGAET2	69.55	69.55	109.83	109.83
ASGAME	83.50	83.50	85.75	85.75
ASGAME2	81.25	81.25	91.00	91.00
ASGAMEH	93.75	93.75	84.73	84.73
ASH	61.75	61.75	50.20	50.20
ASH2	42.25	42.25	46.45	46.45
ASH3	16.63	16.63	55.65	55.65
ASME	59.20	59.20	63.80	63.80
ASME2	34.20	34.20	79.50	79.50
ASME3	2.93	2.93	85.78	85.78
B	133.80	133.80	36.65	36.64
B(S)	0.00	0.00	1.41	1.41
BCL	33.80	33.80	50.94	50.94
BCL2	-19.00	-19.00	65.14	65.15
BCL3	-96.31	-96.31	69.33	69.33
BE	78.25	78.25	32.54	32.54
BE(S)	0.00	0.00	2.28	2.28
BE2SIO4(S)	-506.03	-506.03	15.34	15.33
BE3B2O6(S)	-741.96	-741.96	24.00	23.97
BE3N2(A)	-140.60	-140.60	8.16	8.15
BE3N2(L)	-116.40	-116.41	9.43	9.41
BEAL2O4(S)	-549.90	-549.90	15.84	15.84
BEB2O4	-323.00	-323.00	78.08	78.08
BEBO2	-115.20	-115.20	63.40	63.41
BEBR	28.71	28.71	54.59	54.59
BEBR2	-54.80	-54.80	65.44	65.44
BEBR2(S)	-85.00	-85.00	24.00	23.99
BECL	14.50	14.50	51.98	51.98
BECL2	-86.10	-86.10	60.26	60.26
BECL2(A)	-117.34	-117.34	19.76	19.75
BECL2(B)	-118.60	-118.60	18.12	18.11
BECLF	-137.00	-137.00	58.89	58.89
BEF	-40.60	-40.60	49.15	49.14
BEF2	-190.25	-190.25	54.36	54.36
BEF2(L)	-244.27	-244.28	14.32	14.32
BEH	76.77	76.77	42.24	42.23
BEH+	276.40	276.40	40.76	40.75

Species	$H^o(298)\text{kcal/mole}$		$S^o(298)\text{cal/(mole}\cdot\text{K)}$	
	Data	Fit	Data	Fit
BEH2	30.00	30.00	41.35	41.33
BEH2O2	-161.70	-161.70	55.89	55.91
BEH2O2(A)	-215.80	-215.81	12.80	12.78
BEH2O2(B)	-216.50	-216.51	12.00	11.98
BEI	40.63	40.63	56.69	56.69
BEI2	-15.30	-15.30	69.65	69.65
BEI2(S)	-45.10	-45.11	28.80	28.78
BEN	101.98	101.98	49.87	49.87
BEO(A)	-145.40	-145.39	3.29	3.31
BEO(B)	-143.80	-143.79	3.97	3.99
BEOH	-27.40	-27.40	50.07	50.07
BES(S)	-56.00	-56.00	8.85	8.84
BESO4(A)	-287.00	-287.01	18.64	18.60
BESO4(B)	-286.73	-286.75	18.94	18.91
BESO4(GAM)	-282.06	-282.07	24.09	24.06
BN	-59.97	-59.97	3.54	3.53
C	171.29	171.29	37.76	37.76
C(S)	0.00	0.00	1.37	1.37
C+	432.47	432.02	36.94	36.93
C-	140.61	140.61	36.16	36.16
C2	200.22	200.23	47.63	47.63
C2-	106.00	106.00	46.96	46.96
C2CL3	54.37	54.36	79.93	79.89
C2CL5	7.38	7.39	94.52	94.75
C2CL6	-32.43	-32.44	93.15	93.04
C2F6	-321.20	-321.20	79.37	79.38
C2H	135.00	135.00	51.10	49.55
C2H2	54.19	54.19	48.00	48.01
C2H3	0.00	68.41	0.00	55.32
C2H4	12.54	12.54	52.40	52.37
C2H5	0.00	28.01	0.00	60.13
C2H6	0.00	-20.04	0.00	54.72
C2HCL	51.10	51.10	57.81	57.82
C2HCL5	-35.19	-35.19	91.61	91.51
C2N	133.00	133.00	55.16	55.16
C2N2	73.87	73.87	57.71	57.72
C2O	68.50	68.50	55.68	55.67

Species	$H^o(298)\text{kcal/mole}$		$S^o(298)\text{cal/(mole}\cdot\text{K)}$	
	Data	Fit	Data	Fit
C3	196.00	196.00	56.68	56.66
C3H2	129.39	129.60	62.01	64.81
C3H2(S)	141.43	141.43	59.74	59.75
C3H4	47.67	47.63	57.99	57.94
C3H4C	67.99	68.00	57.94	57.95
C3H4P	45.77	45.77	58.89	58.89
C3H6	0.00	4.89	0.00	61.51
C3H8	0.00	-24.82	0.00	64.56
C3O2	-22.38	-22.38	65.96	65.96
C4	232.00	232.00	54.54	54.55
C4H	0.00	155.08	0.00	60.89
C4H10	-32.02	-31.84	70.94	71.79
C4H2	0.00	111.70	0.00	59.77
C4H6	0.00	34.96	0.00	68.16
C4H8	0.00	-0.13	0.00	73.55
C5	234.00	234.01	57.81	57.82
C5H	0.00	185.99	0.00	62.20
C5H12	0.00	-34.98	0.00	83.48
C5H2	0.00	165.23	0.00	63.69
C5H5	63.83	63.84	68.10	68.13
C5H6	0.00	31.99	0.00	64.45
C6H	0.00	213.15	0.00	74.10
C6H10	0.00	-1.00	0.00	74.75
C6H14	0.00	-39.91	0.00	92.87
C6H2	0.00	169.66	0.00	70.92
C6H3	0.00	158.45	0.00	76.30
C6H4	99.66	99.67	68.25	68.26
C6H5	79.42	79.43	69.81	69.82
C6H5(L)	140.58	140.58	83.39	84.26
C6H5O	10.34	10.35	74.86	74.87
C6H5OH	-25.13	-25.01	76.96	76.93
C6H6	0.00	19.81	0.00	64.35
C6H7	47.94	47.96	73.07	73.07
C8H	0.00	288.86	0.00	78.39
C8H2	0.00	226.15	0.00	75.94
CA	42.85	42.85	36.99	36.98
CA(A)	0.00	0.00	9.93	9.93

Species	$H^o(298)\text{kcal/mole}$		$S^o(298)\text{cal/(mole}\cdot\text{K)}$	
	Data	Fit	Data	Fit
CA(B)	0.12	0.12	10.15	10.15
CA(L)	2.61	2.60	12.11	12.10
CA+	185.30	185.30	38.37	38.37
CA2	82.66	82.66	61.29	61.29
CABR	-11.81	-11.81	60.42	60.41
CABR2	-92.00	-92.00	75.20	75.20
CABR2(S)	-163.30	-163.30	31.00	30.99
CACL	-25.00	-25.00	57.71	57.71
CACL2	-112.70	-112.70	69.35	69.35
CACL2(S)	-190.20	-190.20	25.00	24.99
CAF	-65.00	-65.00	54.86	54.86
CAF2	-187.50	-187.50	65.41	65.42
CAH2O2	-145.98	-145.97	68.23	68.25
CAH2O2(S)	-235.68	-235.68	19.93	19.93
CAI	-1.21	-1.21	62.43	62.42
CAI2	-61.70	-61.70	78.26	78.26
CAO	10.50	10.50	52.49	52.52
CAO(S)	-151.79	-151.79	9.13	9.15
CAOH	-46.34	-46.34	56.25	56.26
CAOH+	88.21	88.21	54.92	54.93
CAS	29.54	29.52	55.56	55.55
CCL	106.10	106.10	52.46	52.45
CCL2	53.02	53.02	63.29	63.28
CCL2CCLO	-24.27	-24.27	85.06	84.97
CCL2CCLOH	-44.66	-44.69	83.09	82.88
CCL2CH	62.30	62.29	71.95	71.93
CCL2HOO	-1.37	-1.33	78.30	79.17
CCL2OHCH2	-22.77	-22.60	79.91	80.63
CCL2OHCHCL	-31.69	-31.54	87.57	89.10
CCL3	16.58	16.58	72.20	72.20
CCL3CCLH2	-35.29	-35.28	85.57	85.59
CCL3CCLO	-56.49	-56.47	89.99	90.43
CCL3CH2	18.79	18.89	81.61	82.80
CCL3CHCL	11.06	11.09	88.40	89.03
CCL3CHO	-45.51	-45.47	83.71	85.04
CCL3OO	-0.74	-0.71	83.14	83.46
CCL4	-20.22	-20.22	78.91	78.91

Species	$H^o(298)\text{kcal/mole}$		$S^o(298)\text{cal/(mole}\cdot\text{K)}$	
	Data	Fit	Data	Fit
CCLH2OO	1.22	1.27	71.06	71.68
CH	142.00	142.00	43.72	43.71
CH+	388.80	388.80	41.00	41.00
CH2	92.48	92.48	46.72	46.71
CH2(S)	101.50	101.50	45.10	45.10
CH2CCL	61.43	61.39	64.24	64.15
CH2CCL2	0.75	0.71	68.84	68.76
CH2CCLOH	-37.01	-36.94	69.00	69.35
CH2CHCCH	69.14	69.14	66.49	67.33
CH2CHCCH2	74.11	74.14	74.70	75.31
CH2CHCH2	38.70	38.64	64.39	64.73
CH2CHCHCH	86.13	86.09	72.75	73.06
CH2CHCHCH2	28.33	28.29	69.74	70.44
CH2CHCL	4.69	4.67	63.03	62.98
CH2CL	27.08	27.07	59.28	59.28
CH2CL2	-22.83	-22.83	64.57	64.57
CH2CLCCL2	6.02	6.05	82.70	83.32
CH2CLCCLO	-58.33	-58.30	77.51	78.10
CH2CLCH2	23.00	23.10	68.36	69.46
CH2CLCH2CL	-32.35	-32.33	72.20	72.45
CH2CLCHCL	13.10	13.14	75.92	76.80
CH2CLCHCL2	-35.23	-35.22	80.05	80.12
CH2CLCHO	-41.67	-41.66	72.11	74.04
CH2CO	0.00	-12.40	0.00	57.78
CH2F2	-107.71	-107.71	58.94	58.91
CH2HCO	0.00	6.00	0.00	63.99
CH2O	-27.70	-27.70	52.26	52.24
CH2OH	-4.21	-4.10	58.93	58.87
CH2OHCCL2	-23.26	-23.21	82.18	82.65
CH2OHCHCL	-16.90	-16.79	74.35	74.94
CH2SICL	45.68	45.67	69.39	69.33
CH2SICL3	-87.71	-87.71	90.16	91.94
CH2SIH2CL	-0.90	-0.87	74.23	75.92
CH2SIHCL2	-44.67	-44.67	83.30	85.08
CH3	34.82	34.82	46.38	46.37
CH3C(O)CL	-56.93	-56.86	70.60	71.87
CH3CC	123.81	123.82	60.28	60.27



Species	$H^o(298)\text{kcal/mole}$		$S^o(298)\text{cal/(mole}\cdot\text{K)}$	
	Data	Fit	Data	Fit
CH3CCCH2	74.33	74.34	78.57	80.35
CH3CCCH3	40.92	40.94	71.58	73.36
CH3CCH2	61.04	61.09	69.12	69.24
CH3CCL	61.68	61.73	66.18	67.81
CH3CCL2	10.33	10.42	75.42	76.27
CH3CCL3	-33.55	-33.51	76.48	76.61
CH3CCLO	-56.93	-56.86	70.60	71.87
CH3CH2CCH	44.66	44.75	71.46	71.43
CH3CH2CH2CH3	-30.64	-30.50	72.68	73.31
CH3CH2CL	-27.17	-27.10	66.00	66.33
CH3CH2O	-0.51	-0.44	65.48	65.81
CH3CHCH	64.70	64.75	68.49	68.74
CH3CHCL	18.22	18.30	68.46	69.48
CH3CHCL2	-32.08	-32.02	72.79	73.04
CH3CHOH	-14.34	-14.17	66.73	67.77
CH3CL	-20.00	-20.00	55.99	55.97
CH3CO	0.00	-5.40	0.00	63.73
CH3F	-56.00	-56.00	53.25	53.22
CH3HCO	0.00	-39.51	0.00	63.04
CH3NO	18.88	18.95	62.33	63.46
CH3NO2	-16.83	-16.84	70.26	72.03
CH3O	0.00	3.89	0.00	54.60
CH3OCH3	-43.80	-43.72	63.74	64.35
CH3OCL	-14.06	-13.98	64.97	65.42
CH3OH	0.00	-48.06	0.00	57.27
CH3ONO	-15.30	-15.25	66.63	66.87
CH3ONO2	-26.12	-26.06	71.34	71.63
CH3SICL	-2.47	-2.44	70.99	72.63
CH3SIH2SIH	-10.12	-9.96	88.03	91.66
CH3SIH2SIH2CH3	-10.92	-10.79	88.03	90.60
CH3SIHCL2	-93.81	-93.74	79.61	80.53
CH4	-17.90	-17.90	44.49	44.46
CHCL	80.00	80.00	56.12	56.11
CHCL2	19.51	19.51	65.08	65.08
CHCL2CCL2	8.53	8.53	90.99	92.74
CHCL2CCLO	-57.87	-57.85	84.59	85.22
CHCL2CH2	20.23	20.24	78.03	79.99

Species	$H^o(298)\text{kcal/mole}$		$S^o(298)\text{cal/(mole}\cdot\text{K)}$	
	Data	Fit	Data	Fit
CHCL2CHCL	10.32	10.35	82.79	83.54
CHCL2CHCL2	-36.03	-36.02	85.18	85.39
CHCL3	-23.25	-23.25	70.64	70.64
CHCLCCL	55.99	55.98	72.48	72.40
CHCLCCLOH	-43.59	-43.51	76.26	76.42
CHCLCH	64.77	64.81	64.47	64.48
CHCLCHCL	-1.15	-1.15	69.24	69.19
CHCLCHOH	-38.64	-38.56	68.93	69.13
CHCLOH	-16.71	-16.65	65.30	65.41
CHCLOHCH2	-15.20	-15.08	74.53	76.30
CHCLOHCHCL	-24.95	-24.85	82.31	83.81
CHF	30.00	30.00	53.36	53.35
CHF3	-166.60	-166.60	62.03	62.02
CHOHCLCCL2	-31.95	-31.84	88.72	90.27
CHSICL	89.13	89.13	70.30	70.30
CHSICL2	29.60	29.61	81.07	82.86
CHSICL3	-35.28	-35.27	88.41	90.19
CHSIH2CL	50.52	50.55	73.11	74.85
CHSIHCL	67.86	67.93	70.62	72.26
CHSIHCL2	7.19	7.22	80.87	82.62
CL	28.99	28.99	39.45	39.45
CL(CH3)SICH2	-13.11	-13.08	78.44	79.58
CL2	0.00	0.00	53.29	53.29
CL2CCCL2	-5.66	-5.67	81.51	81.41
CL2CCHCL	-3.95	-3.96	77.64	77.54
CL2CCHO	-12.45	-12.46	77.67	77.57
CL2CHOH	-66.56	-66.41	71.53	72.50
CL2CO	-52.70	-52.70	67.64	67.64
CL2COH	-22.80	-22.68	73.07	73.68
CL2HCO	-4.12	-4.12	71.65	71.64
CL2SI(CH3)2	-113.74	-113.59	88.72	90.45
CL2SI(CH3)CH2	-64.26	-64.18	92.21	94.86
CL2SICH2	-34.22	-34.25	75.18	75.10
CL2SICH3	-52.78	-52.71	80.76	81.74
CL2SISI	32.71	32.71	79.88	79.88
CL2SISICL	-24.42	-24.41	92.40	92.46
CL2SISICL2	-95.69	-95.69	102.08	102.02

Species	$H^{\circ}(298)\text{kcal/mole}$		$S^{\circ}(298)\text{cal/(mole}\cdot\text{K)}$	
	Data	Fit	Data	Fit
CL3CCO	1500.00	1500.02	-5.27	87.34
CL3CO	-4.37	-4.37	78.35	78.35
CL3COH	-66.33	-66.23	77.64	79.21
CL3SICH3	-137.81	-137.74	84.47	85.28
CL3SISI	-26.17	-26.17	89.43	89.43
CL3SISICL	-99.56	-99.55	101.49	103.27
CLCCCL	56.20	56.20	64.28	64.28
CLCCO	42.24	42.25	68.92	68.87
CLCH2OH	-55.49	-55.49	69.49	71.45
CLCO	-6.48	-6.48	64.39	64.39
CLCOH	1.17	1.13	62.43	62.37
CLH2CO	-2.35	-2.35	64.42	64.41
CLHCO	-44.30	-44.30	61.80	61.79
CLO	29.20	29.19	53.00	52.99
CLOCL	19.71	19.71	63.65	63.65
CLOO	33.60	33.60	63.54	63.53
CLSI(CH3)2	-26.19	-26.06	82.72	84.80
CLSI(CH3)2CH2	-37.20	-37.04	92.86	96.44
CLSI(CH3)3	-86.29	-86.08	90.84	93.65
CLSICH3	-2.86	-2.82	70.99	72.64
CLSISI	99.11	99.11	71.44	71.44
CLSISICL	33.48	33.48	81.76	81.88
CN	104.00	104.00	48.41	48.40
CN+	430.87	430.87	50.99	50.98
CN-	14.50	14.50	46.81	46.81
CN2	113.00	113.00	54.04	54.03
CNN	139.70	139.70	55.35	55.35
CNO	97.64	97.64	55.57	55.57
CO	-26.42	-26.42	47.21	47.21
CO2	-94.05	-94.05	51.07	51.07
CO2-	-105.50	-105.50	57.49	57.48
COS	-33.08	-33.08	55.32	55.33
CS	67.00	67.00	50.30	50.29
CS2	27.95	27.95	56.85	56.85
CSICL	146.05	146.06	68.07	68.07
CSICL2	89.11	89.11	76.71	76.71
CSICL3	9.05	9.05	86.79	86.79

Species	$H^o(298)\text{kcal/mole}$		$S^o(298)\text{cal/(mole}\cdot\text{K)}$	
	Data	Fit	Data	Fit
CSIH2CL	105.85	105.85	69.88	69.88
CSIHCL	119.47	119.47	67.68	67.68
CSIHCL2	63.16	63.16	77.47	77.47
D	52.99	52.99	29.46	29.45
D2	0.00	0.00	34.62	34.62
DH	0.08	0.08	34.34	34.34
DIOXANE	-75.11	-75.12	71.76	71.72
E	0.00	0.00	0.00	4.98
F	18.90	18.90	36.15	36.14
F-	-61.08	-61.08	34.77	34.76
F2	-0.09	-0.09	48.14	48.14
F2N2(C)	16.40	16.40	62.07	62.08
F2O2	14.00	13.99	64.42	64.33
F2SINH	-146.95	-146.93	70.92	70.92
F3SIN	-200.02	-200.02	73.86	73.87
FNNF	17.88	17.88	63.07	63.47
FNO3	2.50	2.50	69.99	69.99
FO	26.00	26.00	51.77	51.76
FO2	3.00	3.00	61.90	61.90
FONO(C)	10.18	10.16	64.43	64.34
FONO(T)	14.13	14.12	64.88	64.79
FSIN	54.37	54.37	63.67	63.67
GA	68.53	68.52	43.83	43.82
GA2H6	31.50	31.50	69.05	69.05
GAAS	88.40	88.40	63.23	63.23
GAAS(3,C)	245.75	245.75	100.00	100.00
GAAS(3,L)	256.25	256.25	127.75	127.75
GAAS(5,C)	357.75	357.75	130.50	130.50
GAAS(5,L)	420.00	420.00	193.50	193.50
GAET	17.75	17.75	81.60	81.60
GAET2	4.50	4.50	100.43	100.43
GAET3	-17.05	-17.05	112.98	112.98
GAH	54.80	54.80	49.18	49.17
GAH2	41.00	41.00	56.00	56.00
GAH3	27.00	27.00	54.50	54.50
GAME	18.53	18.53	63.80	63.80
GAME2	16.42	16.43	80.55	80.55

Species	$H^{\circ}(298)\text{kcal/mole}$		$S^{\circ}(298)\text{cal/(mole}\cdot\text{K)}$	
	Data	Fit	Data	Fit
GAME3	-10.88	-10.87	87.88	87.88
H	52.10	52.09	27.39	27.39
H(CH3)SiCH2	26.36	26.39	70.27	71.37
H+	367.17	367.15	26.01	26.01
H-	33.23	33.19	26.02	26.01
H2	0.00	0.00	31.21	31.21
H2ALME	6.00	6.00	61.73	61.73
H2ASME	24.05	24.05	64.85	64.85
H2C4O	54.58	54.59	66.42	66.43
H2CCC	160.67	160.67	61.07	61.07
H2CCC(S)	133.42	133.42	58.50	58.49
H2CCCCCH	128.19	128.19	75.36	75.37
H2CCCCCH	111.34	111.32	72.83	72.94
H2CCCCCH2	75.53	75.49	64.77	65.12
H2CCCH	83.03	83.04	61.48	61.48
H2CCCLO	-11.53	-11.54	69.74	69.67
H2CCH(SiCl2H)	-66.26	-66.22	84.68	85.71
H2CCH2OH	-4.57	-4.46	69.01	71.17
H2CCHO	3.55	3.51	61.95	61.87
H2CCHSi	97.77	97.77	66.01	65.94
H2CCHSiH	73.54	73.58	66.68	66.79
H2CCHSiH2	58.21	58.21	69.03	68.94
H2CCHSiH3	20.65	20.70	68.95	69.47
H2CLSiCH3	-50.13	-50.06	72.04	73.01
H2CLSiSiCl3	-146.58	-146.56	100.61	101.70
H2CN	59.10	59.11	53.59	53.59
H2CNCH2	56.61	56.53	61.18	61.01
H2CNCH2O	45.02	44.98	68.50	68.38
H2CNCHO	-0.52	-0.56	66.78	66.64
H2CNH	21.89	21.85	54.81	55.45
H2CNNHO	49.78	49.72	67.28	67.10
H2CNNO	58.35	58.36	66.42	66.98
H2CNNO2	33.62	33.64	72.48	73.06
H2CNO	41.46	41.42	61.08	61.01
H2CNO2	36.44	36.47	65.53	65.58
H2CONO	33.07	33.10	68.31	68.54
H2GAET	-2.30	-2.30	83.68	83.68

Species	$H^o(298)\text{kcal/mole}$		$S^o(298)\text{cal/(mole}\cdot\text{K)}$	
	Data	Fit	Data	Fit
H2GAME	15.00	15.00	64.85	64.85
H2NF	-6.49	-6.49	54.73	54.72
H2NNO	18.25	18.21	60.27	60.18
H2NO	15.82	15.82	55.69	55.68
H2NOH	-12.23	-12.16	56.04	56.17
H2O	-57.80	-57.80	45.11	45.10
H2O(L)	0.00	-68.31	0.00	16.71
H2O(S)	0.00	-69.96	0.00	10.71
H2O2	0.00	-32.53	0.00	55.65
H2S	-4.90	-4.90	49.15	49.14
H2SI(CH3)2	-23.20	-23.08	72.44	73.83
H2SI(CH3)CH2	25.55	25.61	77.77	79.83
H2SI(NH2)2	-37.30	-37.15	71.62	72.38
H2SIC	167.19	167.19	60.31	60.21
H2SICCH	90.95	90.95	66.92	66.80
H2SICH	105.35	105.42	62.48	63.58
H2SICH2	40.75	40.72	59.94	59.85
H2SICH3	33.05	33.11	64.52	65.41
H2SIN	149.19	149.19	59.51	59.51
H2SINH	40.99	40.95	59.90	60.09
H2SINH2	28.03	28.09	65.77	65.79
H2SINH3	23.78	23.85	66.78	66.78
H2SISIH2	62.90	62.87	66.69	66.89
H3ASGAET3	-11.00	-11.00	124.48	124.48
H3ASGAME3	-4.70	-4.70	102.50	102.50
H3CONHO	6.46	6.56	71.67	72.65
H3SIC	147.61	147.61	61.79	61.71
H3SICCH	53.02	53.02	64.11	64.02
H3SICH	92.67	92.67	65.63	66.94
H3SICH2	41.54	41.54	67.62	68.97
H3SICH3	-7.32	-7.25	61.75	62.43
H3SIN	234.59	234.60	56.93	56.93
H3SINH	51.32	51.34	65.52	66.21
H3SISIH	74.91	74.96	67.99	69.32
H3SISIH3	19.11	19.16	68.06	68.06
HALME	27.25	27.25	62.78	62.78
HALME2	-6.73	-6.72	75.32	75.33

Species	$H^{\circ}(298)\text{kcal/mole}$		$S^{\circ}(298)\text{cal/(mole}\cdot\text{K)}$	
	Data	Fit	Data	Fit
HASALME	56.50	56.50	83.68	83.68
HASGAET	69.15	69.15	97.28	97.28
HASGAME	70.00	70.00	87.88	87.88
HASME	42.58	42.58	65.90	65.90
HASME2	18.10	18.10	78.45	78.45
HCCCHCCH	134.95	134.95	73.15	73.17
HCCCL	54.95	54.95	57.29	57.29
HCCHCCH	129.91	129.88	68.80	69.06
HCCO	42.44	42.44	60.74	60.73
HCCOH	20.42	20.43	58.69	58.70
HCCSICL2H	-31.76	-31.76	82.04	82.04
HCL	-22.06	-22.06	44.65	44.64
HCL2SICH3	-94.23	-94.16	79.61	80.53
HCL2SISICL2H	-145.25	-145.24	99.80	101.08
HCLCCCLO	-19.42	-19.43	77.51	77.40
HCLCCHO	-6.02	-6.03	70.20	70.09
HCLSI(CH3)2	-68.24	-68.09	81.59	83.53
HCLSI(CH3)CH2	-19.15	-19.06	83.79	86.52
HCLSICH2	2.62	2.59	68.45	68.37
HCLSICH3	-9.10	-9.03	72.91	74.00
HCLSISI	67.05	67.05	71.34	71.34
HCN	31.89	31.89	48.21	48.21
HCNH	66.15	66.10	55.58	55.90
HCNO	38.42	38.43	53.75	53.79
HCO	10.40	10.40	53.67	53.65
HCO+	199.10	199.10	48.59	48.59
HCOOH	-92.57	-92.61	59.32	59.26
HE	0.00	0.00	0.00	30.12
HE+	0.00	568.46	0.00	31.50
HF	-65.14	-65.14	41.51	41.50
HG2BR2(S)	-48.80	-48.80	52.28	52.27
HG2CL2(S)	-63.32	-63.32	46.02	46.00
HG2F2(S)	-116.00	-116.00	38.40	38.39
HG2I2(S)	-28.46	-28.47	57.67	57.66
HGAET	22.90	22.90	83.68	83.68
HGAET2	-2.30	-2.30	100.50	100.50
HGAME	29.00	29.00	65.90	65.90

Species	$H^o(298)\text{kcal/mole}$		$S^o(298)\text{cal/(mole}\cdot\text{K)}$	
	Data	Fit	Data	Fit
HGAME2	2.50	2.50	79.50	79.50
HGBR	24.90	24.90	64.88	64.87
HGCL2	-34.97	-34.96	70.43	70.43
HGCL2(S)	-55.00	-55.00	34.54	34.53
HGF2	-70.19	-70.18	63.55	63.55
HGF2(S)	-101.00	-101.00	27.80	27.79
HGH	57.00	57.00	52.49	52.48
HGI	31.90	31.90	67.07	67.06
HGO	10.00	10.00	57.13	57.13
HGO(S)	-21.70	-21.70	16.80	16.79
HMEGAET	4.00	4.00	88.90	88.90
HN(OH)2	-24.72	-24.64	61.98	62.09
HN3	71.87	71.87	239.08	57.14
HNC	43.85	43.85	48.93	48.93
HNCN	76.43	76.43	59.36	59.36
HNCNH	35.61	35.71	57.31	57.42
HNCO	-28.22	-28.22	57.05	57.05
HNH	32.00	32.00	54.98	54.97
HNH2	-13.79	-13.79	60.06	60.06
HNNHO	21.91	21.86	58.70	58.63
HNNO	55.25	55.20	60.59	60.53
HNNONO	59.02	58.99	70.98	70.97
HNO	23.80	23.80	52.73	52.72
HNO2	-14.15	-14.15	56.75	56.73
HNO3	-32.10	-32.10	63.66	63.66
HNOH	21.05	21.06	55.78	55.78
HO2	2.50	2.50	54.73	54.72
HOCH2OH	-96.64	-96.53	61.14	61.31
HOCL	-18.64	-18.64	56.34	56.33
HOCN	-3.55	-3.53	57.66	59.25
HOCO	-46.31	-46.29	60.12	60.11
HONO	-18.34	-18.34	59.59	59.58
HONO2	-30.18	-30.18	63.20	63.16
HSI(CH3)2	18.27	18.38	74.81	76.56
HSI(CH3)2CH2	9.32	9.44	86.18	88.89
HSI(CH3)3	-39.40	-39.24	83.61	85.87
HSI(NH2)2	5.62	5.77	72.56	73.38



Species	$H^o(298)\text{kcal/mole}$		$S^o(298)\text{cal/(mole}\cdot\text{K)}$	
	Data	Fit	Data	Fit
HSI(NH <sub>2</sub> ) <sub>3</sub>	-64.86	-64.68	78.65	79.52
HSIC	184.85	184.85	58.24	58.13
HSICCH	104.97	104.97	64.44	64.32
HSICH <sub>2</sub>	85.83	85.81	60.64	60.53
HSICH <sub>3</sub>	48.84	48.90	62.04	63.21
HSICL	17.00	17.00	59.80	59.80
HSIN	92.99	92.99	54.76	54.75
HSINH	84.80	84.79	60.63	60.68
HSINH <sub>2</sub>	26.33	26.29	59.77	60.05
HSISICL	79.13	79.11	73.04	72.96
I*C <sub>3</sub> H <sub>7</sub>	0.00	18.20	0.00	60.09
K	21.31	21.31	38.30	38.30
K(L)	0.55	0.55	17.08	17.07
K+	122.90	122.90	36.92	36.92
K <sub>2</sub>	30.37	30.37	59.67	59.66
K <sub>2</sub> B <sub>4</sub> O <sub>7</sub> (S)	-796.90	-796.89	49.80	49.82
K <sub>2</sub> B <sub>6</sub> O <sub>10</sub> (S)	-1107.44	-1107.50	60.00	59.87
K <sub>2</sub> B <sub>8</sub> O <sub>13</sub> (S)	-1420.92	-1420.93	70.20	70.18
K <sub>2</sub> CO <sub>3</sub> (S)	-274.90	-274.91	37.17	37.15
K <sub>2</sub> H <sub>2</sub> O <sub>2</sub>	-156.50	-156.50	78.37	78.35
K <sub>2</sub> O(S)	-86.80	-86.79	22.50	22.51
K <sub>2</sub> O <sub>2</sub> (S)	-118.50	-118.47	27.00	27.05
K <sub>2</sub> SO <sub>4</sub>	-261.50	-261.50	87.49	87.50
K <sub>2</sub> SO <sub>4</sub> (A)	-343.62	-343.62	41.96	41.94
K <sub>2</sub> SO <sub>4</sub> (B)	-340.40	-340.41	45.96	45.94
K <sub>3</sub> CL <sub>6</sub> AL(S)	-500.00	-499.97	90.00	90.08
K <sub>3</sub> CL <sub>9</sub> AL <sub>2</sub> (S)	-683.60	-683.61	112.00	111.96
K <sub>3</sub> F <sub>6</sub> AL(S)	-795.00	-794.96	68.00	68.11
KBF <sub>4</sub>	-371.00	-371.00	75.35	75.36
KBO <sub>2</sub>	-161.10	-161.10	71.06	71.06
KBO <sub>2</sub> (S)	-237.80	-237.81	19.12	19.10
KBR	-43.04	-43.04	59.85	59.85
KBR(L)	-89.98	-89.99	25.23	25.22
KBR(S)	-94.12	-94.12	22.93	22.92
KCL	-51.31	-51.31	57.12	57.11
KCL(L)	-100.81	-100.81	20.71	20.71
KCL(S)	-104.37	-104.37	19.73	19.73

Species	$H^o(298)\text{kcal/mole}$		$S^o(298)\text{cal/(mole}\cdot\text{K)}$	
	Data	Fit	Data	Fit
KCL4AL(S)	-286.00	-286.01	47.00	46.98
KCLO4(S)	-102.80	-100.21	36.10	40.62
KCN	19.00	19.00	60.48	60.47
KCN(L)	-24.89	-24.89	32.10	32.09
KCN(S)	-27.12	-27.12	30.54	30.53
KF	-78.10	-78.10	54.14	54.13
KF(L)	-132.52	-132.52	16.17	16.16
KF(S)	-135.90	-135.90	15.91	15.91
KH	29.40	29.40	47.30	47.30
KH(S)	-13.82	-13.81	12.00	12.02
KI	-30.00	-30.00	61.70	61.70
KI(L)	-74.77	-74.77	27.27	27.26
KI(S)	-78.37	-78.37	25.43	25.42
KO	17.00	17.00	56.86	56.86
KO-	-33.00	-33.00	54.06	54.06
KO2(S)	-68.00	-68.00	29.28	29.27
KOH	-98.64	-98.65	23.09	23.07
KOH+	119.00	119.00	59.80	59.81
ME2GAET	-5.25	-5.25	97.28	97.28
MEGAET	14.25	14.25	89.95	89.95
MEGAET2	-7.33	-7.32	106.70	106.71
MG	35.28	35.28	35.50	35.50
MG(L)	2.16	2.16	10.16	10.16
MG(S)	0.00	0.00	7.81	7.81
MG+	213.09	213.09	36.88	36.88
MG2	68.91	68.91	58.28	58.27
MG2BR4	-183.50	-183.50	110.24	110.23
MG2C3(S)	19.00	19.00	24.00	24.01
MG2F4	-410.70	-410.69	80.52	80.55
MGAL2O4(S)	-549.50	-549.49	21.20	21.22
MGB2(S)	-21.98	-21.99	8.60	8.59
MGBR	-8.45	-8.45	58.52	58.52
MGBR2	-72.40	-72.40	71.92	71.92
MGBR2+	174.80	174.80	76.87	76.87
MGC2(S)	21.00	21.00	13.00	13.01
MGCL	-10.40	-10.40	55.76	55.76
MGCL2	-93.80	-93.80	66.18	66.18

Species	$H^{\circ}(298)\text{kcal/mole}$		$S^{\circ}(298)\text{cal/(mole}\cdot\text{K)}$	
	Data	Fit	Data	Fit
MGCL2(S)	-153.35	-153.35	21.42	21.42
MGCO3(S)	-265.70	-265.70	15.74	15.73
MGF	-56.60	-56.60	52.81	52.81
MGF2	-173.70	-173.70	61.28	61.28
MGF2(S)	-268.70	-268.70	13.68	13.67
MGF2+	141.49	141.49	61.67	61.68
MGH	40.40	40.40	46.15	46.14
MGH2(S)	-18.20	-18.20	7.43	7.42
MGH2O2	-136.80	-136.80	63.85	63.87
MGH2O2(S)	-221.00	-221.00	15.12	15.10
MGN	69.00	69.00	53.71	53.71
MGO(S)	-143.70	-143.70	6.44	6.45
MGOH	-39.38	-39.38	54.10	54.11
MGOH+	139.68	139.68	52.75	52.76
MGS	34.71	34.71	53.87	53.84
MGS(S)	-82.63	-82.63	12.03	12.02
MGSO4(S)	-301.57	-301.58	21.84	21.83
N	112.98	112.95	36.61	36.61
N*C3H7	0.00	22.60	0.00	64.13
N2	0.00	0.00	45.77	45.76
N2F2(C)	17.88	17.88	62.26	62.24
N2F2(T)	20.08	20.07	62.14	62.06
N2F4	-2.00	-2.00	71.96	71.98
N2H2	50.90	50.90	52.22	52.20
N2H3	0.00	36.78	0.00	54.61
N2H4	22.79	22.79	57.03	57.02
N2H4(L)	12.10	12.09	29.05	29.03
N2O	19.61	19.61	52.55	52.55
N2O+	318.69	318.69	55.87	55.86
N2O4	2.17	2.17	72.72	72.72
N3	99.00	99.00	54.10	54.10
NA	25.76	25.75	36.71	36.71
NA(L)	0.58	0.57	13.83	13.82
NA+	145.76	145.75	35.34	35.33
NA2	32.87	32.87	54.99	54.99
NA2B4O7(S)	-783.16	-783.17	45.29	45.27
NA2B6O10(S)	-1094.76	-1094.79	55.50	55.43

Species	$H^o(298)\text{kcal/mole}$		$S^o(298)\text{cal/(mole}\cdot\text{K)}$	
	Data	Fit	Data	Fit
NA2C2N2	-2.10	-2.10	82.93	82.93
NA2F2	-202.30	-202.30	68.66	68.67
NA2H2O2	-145.20	-145.20	73.44	73.43
NA2O(L)	-89.11	-89.12	21.90	21.88
NA2O(S)	-99.90	-98.48	17.94	19.10
NA2O2	-122.66	-121.57	22.66	24.05
NA2SO4	-247.04	-247.04	82.87	82.89
NA2SO4(D)	-329.66	-329.66	39.01	38.99
NA2SO4(i)	-330.04	-330.04	38.30	38.28
NA2SO4(iii)	-330.99	-330.99	37.02	37.01
NA2SO4(iv)	-331.63	-331.64	35.89	35.87
NA2SO4(v)	-331.70	-331.70	35.75	35.74
NA3CL6AL(S)	-473.00	-472.97	83.00	83.08
NA3F6AL(S)	-792.76	-792.77	57.00	56.97
NABH4(S)	-45.85	-45.85	24.23	24.23
NABO2	-155.00	-155.00	68.63	68.63
NABO2(S)	-233.20	-233.21	17.58	17.56
NABR	-34.40	-34.40	57.63	57.63
NABR(L)	-81.11	-81.11	24.94	24.93
NABR(S)	-86.38	-86.38	20.75	20.74
NACH	22.53	22.53	58.14	58.14
NACL	-43.36	-43.36	54.90	54.90
NACL(S)	-98.26	-98.26	17.24	17.23
NACL4AL(S)	-273.00	-273.01	45.00	44.97
NACN	22.53	22.53	58.14	58.14
NACN(S)	-21.68	-21.68	28.32	28.31
NAF	-69.42	-69.42	51.98	51.98
NAF2-	-160.00	-160.00	59.89	59.89
NAF4AL	-440.00	-440.00	82.41	82.43
NAH	29.70	29.70	45.00	44.99
NAI(S)	-68.80	-68.80	23.54	23.54
NAO	20.00	20.00	54.74	54.74
NAO-	-29.00	-29.00	51.95	51.95
NAO2(S)	-62.30	-62.30	27.70	27.69
NAO2AL(S)	-270.84	-270.59	16.83	17.17
NAOH	-47.27	-47.26	54.57	54.58
NAOH(L)	-99.64	-99.64	18.13	18.12

Species	$H^{\circ}(298)\text{kcal/mole}$		$S^{\circ}(298)\text{cal/(mole}\cdot\text{K)}$	
	Data	Fit	Data	Fit
NAOH+	162.00	162.00	57.96	57.96
NCN	107.59	107.59	54.77	54.76
NCO	31.51	31.51	54.14	54.14
NF	53.93	53.93	50.82	50.82
NF2	7.87	7.87	59.40	59.39
NF3	-27.97	-27.97	61.79	61.79
NFO	-15.70	-15.70	59.27	59.27
NFO2	-26.00	-26.00	62.18	62.18
NH	85.20	85.20	43.29	43.29
NH2	45.50	45.50	46.51	46.50
NH3	-10.97	-10.97	46.05	46.03
NNH	58.57	58.57	53.63	53.62
NO	21.58	21.58	50.35	50.34
NO+	236.66	236.66	47.35	47.34
NO2	7.91	7.91	57.34	57.33
NO2-	-48.45	-48.45	56.52	56.51
NO2F	-23.10	-23.09	61.26	61.26
NO3	17.00	17.00	60.35	60.35
NO3F	3.34	3.34	68.94	68.85
NOF	-16.91	-16.90	58.63	58.63
NOF3	-39.00	-39.00	66.54	66.55
O	59.55	59.55	38.47	38.46
O+	374.95	374.95	37.01	37.01
O-	24.32	24.32	37.69	37.68
O2	0.00	0.00	49.01	49.00
O2-	-11.61	-11.62	50.06	50.06
O2F	22.56	22.56	60.57	60.56
O3	34.10	34.10	57.08	57.08
OC(OH)2	-147.04	-147.04	64.46	64.40
OCHCHO	-49.55	-49.53	64.82	64.98
OCHNNHO	-2.05	-2.09	69.36	69.15
OF	23.73	23.73	50.43	50.43
OF2	4.60	4.60	58.54	58.54
OH	9.32	9.32	43.88	43.87
OH+	314.80	314.80	43.66	43.65
OH-	-34.32	-34.32	41.19	41.19
ONHNHO	23.55	23.52	62.66	62.55

Species	$H^o(298)\text{kcal/mole}$		$S^o(298)\text{cal/(mole}\cdot\text{K)}$	
	Data	Fit	Data	Fit
ONHNOH	-1.77	-1.77	65.04	64.93
P	79.80	79.80	38.98	38.98
P2	42.68	42.68	52.11	52.11
P4	30.77	30.78	66.89	66.92
S	66.20	66.20	40.09	40.09
S(L)	0.00	0.44	0.00	8.77
S(S)	0.00	0.00	0.00	7.62
S+	306.48	306.47	39.08	39.08
S-TRIAZINE	56.36	56.37	64.49	64.49
S2	30.71	30.71	54.51	54.50
SH	33.30	33.30	46.73	46.73
SI	107.70	107.70	40.12	40.12
SI(CH3)2	32.16	32.19	74.55	77.23
SI(CH3)3	3.12	3.28	84.75	87.23
SI(CH3)3CH2	-6.88	-6.71	96.57	99.89
SI(CH3)4	-55.74	-55.51	93.08	96.05
SI(L)	11.59	11.58	10.63	10.62
SI(NH2)3	-18.77	-18.63	84.34	84.27
SI(NH2)4	-92.88	-92.67	84.54	85.38
SI(S)	0.00	0.00	4.50	4.50
SI2	145.79	145.79	54.83	54.83
SI2C	128.00	128.00	57.88	57.88
SI2CL5	-151.65	-151.64	109.12	110.10
SI2CL5H	-188.98	-188.97	108.00	108.98
SI2CL6	-232.75	-232.73	111.13	111.85
SI2F6	-569.62	-569.61	97.16	97.16
SI2H2	95.63	95.62	58.84	58.83
SI2H3	105.70	105.70	65.51	65.51
SI2H5	55.70	55.70	68.85	68.85
SI2H6	19.10	19.10	64.54	64.53
SI3	152.00	152.00	64.00	64.01
SI3H8	28.90	28.90	81.57	81.56
SI3N4(A)	-178.00	-178.00	27.00	26.99
SIC	172.00	172.01	50.89	50.93
SIC(B)	-17.50	-17.50	3.97	3.98
SIC2	147.00	147.00	56.55	56.55
SICCH	125.77	125.77	60.40	60.26

Species	$H^{\circ}(298)\text{kcal/mole}$		$S^{\circ}(298)\text{cal/(mole}\cdot\text{K)}$	
	Data	Fit	Data	Fit
SICH	124.39	124.39	54.94	54.83
SICH <sub>2</sub>	74.15	74.15	55.99	55.92
SICH <sub>3</sub>	74.53	74.53	60.16	60.13
SICL	37.90	37.90	56.80	56.80
SICL <sub>2</sub>	-40.30	-40.30	67.20	67.20
SICL <sub>2</sub> H <sub>2</sub>	-74.50	-74.50	68.40	68.40
SICL <sub>3</sub>	-76.50	-76.50	75.50	75.50
SICL <sub>3</sub> CH <sub>2</sub> CH	-140.60	-140.59	93.99	95.65
SICL <sub>3</sub> H	-118.60	-118.60	74.90	74.89
SICL <sub>4</sub>	-158.40	-158.40	79.10	79.09
SICLH <sub>3</sub>	-32.20	-32.20	59.80	59.79
SIF	-12.42	-12.42	52.71	52.71
SIF(NH <sub>2</sub> ) <sub>2</sub>	-95.48	-95.33	76.93	77.70
SIF(NH <sub>2</sub> ) <sub>3</sub>	-170.70	-170.55	87.97	87.91
SIF <sub>2</sub>	-149.86	-149.86	61.38	61.38
SIF <sub>2</sub> (NH <sub>2</sub> ) <sub>2</sub>	-247.30	-247.19	82.82	82.77
SIF <sub>2</sub> N	-63.11	-63.11	70.51	70.51
SIF <sub>2</sub> NH <sub>2</sub>	-167.24	-167.21	77.17	77.48
SIF <sub>3</sub>	-237.42	-237.42	67.76	67.76
SIF <sub>3</sub> NH	-249.65	-249.65	82.15	83.70
SIF <sub>3</sub> NH <sub>2</sub>	-317.89	-317.89	79.98	81.03
SIF <sub>3</sub> NHSIH <sub>3</sub>	-320.19	-320.16	95.97	96.88
SIF <sub>3</sub> NSIH <sub>3</sub>	-252.84	-252.83	97.65	99.34
SIF <sub>4</sub>	-385.98	-385.98	67.55	67.54
SIFH <sub>3</sub>	-85.50	-85.50	57.00	57.00
SIFNH	-13.57	-13.49	68.88	68.95
SIFNH <sub>2</sub>	-80.01	-80.04	64.68	64.62
SIH	91.70	91.70	44.20	44.20
SIH <sub>2</sub>	64.80	64.80	49.50	49.49
SIH <sub>2</sub> CL	7.80	7.80	62.30	62.30
SIH <sub>2</sub> F	-42.16	-42.16	59.70	59.70
SIH <sub>2</sub> F <sub>2</sub>	-186.38	-186.38	62.81	62.81
SIH <sub>3</sub>	47.43	47.43	51.81	51.80
SIH <sub>3</sub> NH <sub>2</sub>	-11.45	-11.40	65.66	65.66
SIH <sub>3</sub> NHSIH <sub>3</sub>	-14.32	-14.32	83.54	85.95
SIH <sub>3</sub> NSIH <sub>3</sub>	48.90	48.90	83.75	86.69
SIH <sub>3</sub> SIH <sub>2</sub> CH <sub>3</sub>	4.03	4.14	79.43	81.90

Species	$H^o(298)\text{kcal/mole}$		$S^o(298)\text{cal/(mole}\cdot\text{K)}$	
	Data	Fit	Data	Fit
SIH4	8.09	8.10	48.90	48.90
SIHCL2	-34.30	-34.30	70.30	70.30
SIHF	-35.70	-35.70	57.07	57.07
SIHF2	-139.57	-139.57	65.05	65.05
SIHF3	-288.63	-288.63	66.65	66.65
SIN	115.55	115.55	51.95	51.95
SINH	38.39	38.39	51.66	51.66
SINH2	48.67	48.67	58.56	58.56
SN	63.00	63.00	53.06	53.05
SO	1.20	1.20	53.02	53.01
SO2	-70.95	-70.95	59.30	59.29
SO3	-94.59	-94.59	61.34	61.34
TI	113.20	113.20	43.07	43.06
TICL	36.90	36.90	59.54	59.54
TICL2	-56.70	-56.70	66.50	66.50
TICL3	-128.90	-128.90	75.70	75.71
TICL4	-182.40	-182.40	84.79	84.80



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## Chapter 3: Gas-phase Kinetics Input

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The *Gas-phase Kinetics* input file provides a symbolic description of an elementary chemical reaction mechanism. This file is used during Pre-processing to create a *Gas-phase Kinetics* linking file (*chem.asc*) that stores pertinent information about that mechanism for access during the reactor-model simulation. The information in the Linking File is subsequently accessed by an initialization routine that copies the needed information into memory during a reacting-flow simulation. The stored information is used in calculations related to the equation of state, thermodynamic properties, and chemical production rates.

The *Gas-phase Kinetics* input file includes information on elements, species, thermodynamic data, and the reaction mechanism. Element data are read first, species data are second, followed by optional thermodynamic data, with reactions specified last. The thermodynamic data for the species may come be included in the *Gas-phase Kinetics* input file and/or from a Thermodynamic Database (e.g., *therm.dat*). With the exception of the thermodynamic data, all input is free format. The required syntax for the four types of input is described in [Element Data \(p. 33\)](#) through [Reaction Mechanism Description \(p. 39\)](#). The auxiliary keywords for gas-phase reactions are described in [Table 3.7: Alphabetical Listing of Gas-phase Reaction Auxiliary Keywords \(p. 43\)](#) and the options for specifying units on the REACTIONS line are described in [Table 3.4: Alphabetical Listing of REACTIONS-line Options for Gas-phase Kinetics Data \(p. 39\)](#). [Alphabetical Listing of Project Input Keywords \(p. 123\)](#) describes the meaning and usage of each keyword entry that may be included as part of a Reactor Model input file.

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### Note:

Input information in the *Gas-phase Kinetics* input file must be contained within the first **100 columns, or it will be ignored.**

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### 3.1. Element Data

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All chemical species in the reaction mechanism must be composed of chemical elements or isotopes of chemical elements. Each element and isotope must be declared as a one- or two-character symbol. The purpose of the element data is to associate atomic weights of the elements with their character symbol representations and to identify the order in which arrays of element information in the *Gas-phase Kinetics* Subroutine Library are referenced. For example, an array of atomic weights for the elements is in exactly the same order in which the elements were declared in the element data. In other words, if the atomic weights are stored in an array AWT, then AWT( 3 ) is the atomic weight of the third element declared in the element data.

Element data must start with the word ELEMENTS (or ELEM), followed by any number of element symbols on any number of lines. Element symbols may appear anywhere on a line, but those on the same line must be separated by blanks. Any line or portion of a line starting with an exclamation mark (!) is considered a comment and will be ignored. Blank lines are ignored.

If an element is on the periodic chart, then only the symbol identifying the element need appear in the element data.

### Note:

The elements that ANSYS Chemkin-Pro recognizes are as follows: H, HE, LI, BE, B, C, N, O, F, NE, NA, MG, AL, SI, P, S, CL, AR, K, CA, SC, TI, V, CR, MN, FE, CO, NI, CU, ZN, GA, GE, AS, SE, BR, KR, RB, SR, Y, ZR, NB, MO, TC, RU, RH, PD, AG, CD, IN, SN, SB, TE, I, XE, CS, BA, LA, CE, PR, ND, PM, SM, EU, GD, TB, DY, HO, ER, TM, YB, LU, HF, TA, W, RE, OS, IR, PT, AU, HG, TL, PB, BI, PO, AT, RN, FR, RA, AC, TH, PA, U, NP, PU, AM, CM, BK, CF, ES, FM, D, E

For the elements appearing on the periodic chart, the ANSYS Chemkin-Pro pre-processors have the atomic weight (in grams per mole) stored internally. For isotopes, a one- or two- character symbol must be input by the user to identify each isotope, and a symbol and an atomic weight (in grams per mole) for each must be defined. The same symbol must be used in the thermodynamic data to identify the elemental composition of species involving the isotope. Once an isotope has been so defined, it is treated exactly as a new element. If an ionic species is used in the reaction mechanism (i.e., OH<sup>+</sup>), an electron must be declared as the element E.

For an isotope, the atomic weight must follow the identifying symbol and be delimited by slashes (/). The atomic weight may be in integer, floating-point, or E format (e.g., 2, 2.0, 0.2E1), but internally it will be converted to a floating point number. For example, the isotope deuterium may be defined as D/2.014/. If desired, the atomic weight of an element in the periodic chart may be altered by including the atomic weight as input just as though the element were an isotope.

Figure 3.1: Examples of Species Data (p. 34) shows several equivalent ways to describe element information. In this example the elements are hydrogen, oxygen, nitrogen, and the isotope deuterium.

**Figure 3.1: Examples of Species Data**

```
ELEMENTS  H  D /2.014/  O  N  END

ELEM                                ! ELEM is equivalent to ELEMENTS
H
D / 2.014 /
O
N
END                                ! an END line is optional

ELEM H
ELEM D/2.014/
ELEM O
ELEM N
```

Table 3.1: Summary of the Rules for Element Data (p. 34) summarizes the rules for element data.

**Table 3.1: Summary of the Rules for Element Data**

Rule	Description
1	The first element line must start with the word ELEMENTS (or ELEM).
2	Element or isotope names are either one- or two-character symbols.
3	An isotope name (i.e., a name not on the periodic chart) must be followed by its atomic weight (in grams per mole) delimited by slashes.

Rule	Description
4	Each element or isotope should be declared only once; however, duplicated element symbols will be ignored.
5	An element or isotope name may appear anywhere on the line.
6	Any number of element or isotope names may appear on a line, and more than one line may be used.
7	Element or isotope names that appear on the same line must be separated by at least one blank space.
8	An element or isotope name that begins on one line may not continue to the next line.
9	Any blank spaces between an element or isotope name and the first slash are ignored and any blank spaces between slashes and an atomic weight are also ignored. However, no blank spaces are allowed within an element name or an atomic weight.
10	There may be more than one ELEMENT statement.
11	All characters following an exclamation mark are comments.
12	It is recommended that an END statement follow a group of elements.
13	Elements required by <i>Surface Kinetics</i> surface species must be declared in the <i>Gas-phase Kinetics</i> input file.

## 3.2. Species Data

Each chemical species in a problem must be identified on one or more species line(s). Any set of up to 16 upper or lower case characters can be used as a species name. In addition each species must be composed of elements that have been identified in the element data. As for the element data, one of the primary purposes of the species data is to identify the order in which arrays of species information are referenced in the *Gas-phase Kinetics* Subroutine Library.

Species data must start with the word SPECIES (or SPEC), followed by any number of species symbols on any number of lines. Species symbols may appear anywhere on a line, but those on the same line must be separated by blank spaces. Any line or portion of a line starting with an exclamation mark (!) is considered to be a comment and will be ignored. Blank lines are ignored. [Figure 3.2: Examples of Species Data \(p. 35\)](#) shows several equivalent ways to describe species information.

**Figure 3.2: Examples of Species Data**

```

SPECIES      H2  O2  H  O  OH  HO2  N2  N  NO  END

SPEC                                     ! SPEC is equivalent to SPECIES
  H2  O2
  H  O  OH  HO2  N2  N  NO
END

SPEC H2
spec O2

```

The rules for species data are summarized in [Table 3.2: Summary of the Rules for Species Data](#) (p. 36).

**Table 3.2: Summary of the Rules for Species Data**

Rule	Description
1	Species data must start with the word <code>SPECIES</code> (or <code>SPEC</code> ).
2	Species names are composed of up to 16-character upper- or lower- case symbols. The names cannot begin with the characters <code>+</code> , <code>=</code> , or a number; an ionic species name may end with one or more <code>+</code> 's or <code>-</code> 's.
3	Each species should be declared only once; however, duplicated species symbols will be ignored.
4	Each species that subsequently appears in a reaction must be declared.
5	A species name may appear anywhere on the line.
6	Any number of species names may appear on a line, and more than one line may be used.
7	Species named on the same line must be separated by at least one blank space.
8	A species name that begins on one line may not continue to the next line.
9	There may be more than one <code>SPECIES</code> statement.
10	All characters following an exclamation mark are comments.
11	For best results, an <code>END</code> statement should follow a species group.

### 3.3. Thermodynamic Data

All gas-phase species that appears in the reactions contained in the *Gas-phase Kinetics* input or in the *Surface Kinetics* input, must have associated thermodynamic data. The data may be extracted from a database file (e.g. *therm.dat*) and/or read directly from the *Gas-phase Kinetics* input file. Details on the thermodynamic data format, whether including in the *Gas-phase Kinetics* input file or in a thermodynamic database file, are provided in [Thermodynamic Data Format](#) (p. 3).

---

#### Note:

When thermodynamic data input is included in the *Gas-phase Kinetics* input file, it must immediately follow species data.

---

#### Note:

The *therm.dat* file distributed with ANSYS Chemkin-Pro represents a historical (not necessarily best) collection of data accumulated by Sandia National Laboratories over the period from 1980 to 1995. The data fits in this collection are based on a variety of sources, including JANAF Tables, NASA, and computational chemistry calculations performed at Sandia and elsewhere. This data set has been fixed and not updated in order to assure backwards compatibility and consistency with published Chemkin-Pro results.

---

### 3.4. Real Gas Data

ANSYS Chemkin-Pro employs the cubic equation of state (EOS) to capture the P-T-V relationship of a real gas mixture at high pressures. For each gas species in the real gas mixture, the cubic equation of state models require additional properties that are not part of the regular thermodynamic data. These properties include the critical point,  $P_c$ ,  $T_c$ , and  $V_c$ , and the acentric factor  $\omega$ , and would be provided in the real gas data block of the gas-phase mechanism. The real gas data block starts with the keyword EOS\_. Immediately following this keyword (no space), a phrase indicating the choice of the cubic equation of state model to be used with this gas mechanism is appended. There are five cubic EOS models available in ANSYS Chemkin-Pro. (For more details, see [Real Gas Model in the Chemkin-Pro Theory Manual](#) ) These cubic equation of state models, along with their key phrases, are listed in [Table 3.3: Cubic equation of state models available in Chemkin-Pro \(p. 37\)](#). For example, the keyword EOS\_PR will cause the Peng-Robinson equation of state to be applied whenever this gas mechanism is used in a ANSYS Chemkin-Pro simulation.

**Table 3.3: Cubic equation of state models available in Chemkin-Pro**

Cubic EOS Model	Key Phrase
van der Waals	<b>VAND</b> or <b>VDW</b>
Redlich-Kwong	<b>REDL</b> or <b>RK</b>
Soave-Redlich-Kwong	<b>SOAV</b> or <b>SRK</b>
Aungier-Redlich-Kwong	<b>AUNG</b> or <b>ARK</b>
Peng-Robinson	<b>PENG</b> or <b>PR</b>

The required properties of all gas species in the mechanism are given below the EOS\_ keyword. Each gas species will have its properties listed in one single line. The line must start with the species name and be followed by, in the exact same order, the values of  $P_c$ ,  $T_c$ ,  $V_c$ , and  $\omega$  for this gas species. The critical pressure  $P_c$  is in bar, the critical temperature  $T_c$  in Kelvin, and the critical molar volume  $V_c$  in  $\text{cm}^3/\text{mole}$ . All four parameters are required. If  $V_c$  or  $\omega$  are not available for a species, set the value to zero.

The parameters are format-free and separated by blank space(s). If the binary interaction coefficients between this gas species and other species are known, the coefficients can be given as auxiliary keywords in the line(s) below the property data line. The interacting species name and the corresponding binary interaction coefficient should be provided in the format illustrated here with the coefficient value delimited by slashes (/):

```
<interacting species name>/<interaction coefficient>/
```

For example, the binary interaction coefficient between O2 and N2 can be given in a line below the properties data line of O2 (or N2) as N2/-0.0078/ (or O2/-0.0078/).

If you have multiple binary interaction coefficients to specify, they should be separated by blank space(s) and can be written in a single line or in several lines. The binary interaction coefficient is only required once for each pair of species.

All species in the mechanism must have their real gas data given in the real gas data block, and the species data lines can appear in any order. The real gas data block should be closed by the keyword END.

[Figure 3.3: Example of Real Gas data input \(p. 38\)](#) shows some examples of the real gas data input.

**Figure 3.3: Example of Real Gas data input**

```

! Real Gas Information
! R.C. Reid, J.M. Prausnitz, and B.E. Poling, The Properties of Gases & Liquids, 4th ED.
EOS_SRK
! Soave-Redlich-Kwong EOS
! Species symbol, TC[K], PC[bar], VC[cm3/mol], Best-fitted Acentric Factor
H      33.2      13.64      0.0      0.0
H2     33.15     13.0      65.1     -0.2324
! Binary Inteaction Coefficients
O      44.5      26.9      0.0      0.0
O2     154.6     50.4     73.4     0.0298
! Binary Inteaction Coefficients
OH     400.0     149.0      0.0      0.1
HO2    400.0     82.0      0.0      0.2
H2O    647.37    221.2     57.1     0.3443
H2O2   730.10    21.68      0.0      0.5
CH4    190.56     46.0     99.2     0.01142
! Binary Inteaction Coefficients
CO2/0.093/ N2/0.028/ CO/0.032/
CO     132.9     35.0     93.2     0.0295
! Binary Inteaction Coefficients
CH4/0.032/
CO2    304.1     73.8     93.9     0.2373
! Binary Inteaction Coefficients
N2/-0.032/
CH4/0.093/
N2     126.2     33.9     89.8     0.0358
! Binary Inteaction Coefficients
CO2/-0.032/ CH4/0.028/
END

```

## 3.5. Transport Data

Gas-phase species transport data is required for a collision-frequency reaction formulation, and for reactor models or other programs that require a transport linkfile. The data can be read from a database file (e.g., *tran.dat*) and/or read directly from the *Gas-phase Kinetics* input file. To include transport data in the input file, the first line of the data should be the word **TRANSPORT** (or **TRAN**), and the last line should be the word **END**. If **TRANSPORT ALL** is used, it is expected that all required transport data is given in this section, or else a database file is used to supplement data not provided here.

The **TRANSPORT . . . END** data block's format should resemble this:

```

TRANSPORT
C2H4 2 280.800 3.971 0.000 0.000 1.500
END

```

For the collision frequency reaction, the required collision diameter of species will be obtained from the transport data and stored in the gas-phase linkfile. For reactor models or other programs that require a supplemental transport linkfile, the User Interface provides a check-box option on the Pre-Processing panel, Process Transport Properties; if this is checked, transport-data coefficient fitting is performed, and a transport linkfile written.

Details on the transport data format, whether included in the *Gas-Phase Kinetics* input file or in a transport properties database file, are provided in [Transport Data Format \(p. 87\)](#).

### Note:

If the *Gas-Phase Kinetics* input file includes transport properties data input, this data must follow species data and precede reaction data.

## 3.6. Reaction Mechanism Description

The reaction mechanism may consist of any number of chemical reactions involving the species named in the species data. A reaction may be reversible or irreversible; it may be a three-body reaction with an arbitrary third body and/or enhanced third-body efficiencies; it may have a Lindemann [4] (p. 345), Troe [5] (p. 345) or SRI [6] (p. 345) pressure fall-off formulation; it may have an arbitrary pressure-dependence defined by special fits or interpolation; it may involve a photon; and it may depend on a species temperature other than that of the bulk gas. [Pressure-dependent Reactions](#) of the [Chemkin-Pro Theory Manual](#) provides more detailed discussion of these different formulations. In this section, we describe the rules and syntax needed to enter different types of reactions in the *Gas-phase Kinetics* input file. The keywords for controlling these reaction parameters are described in [Alphabetical Listing of Project Input Keywords](#) (p. 123) .

Reaction data must start with a line that contains the word REACTIONS (or REAC). The lines following the REACTIONS line contain reaction descriptions, together with their Arrhenius rate coefficients. The reaction description is composed of a reaction path, reaction rate coefficients, and (optionally) some auxiliary information or keywords.

### 3.6.1. REACTIONS Line Options

On the same line as the REACTIONS word, you may specify units of the Arrhenius rate coefficients ([Equation 3.5](#) of the [Chemkin-Pro Theory Manual](#) ) followed by the word CAL/MOLE, KCAL/MOLE, JOULES/MOLE, KJOULES/MOLE, KELVINS, or EVOLTS for  $E_i$ , and/or MOLES or MOLECULES for  $A_i$ . If MOLECULES is specified, then the units for  $A_i$  are cm, molecules, sec, and K.

#### Note:

If units are not specified,  $A_i$  and  $E_i$  must be in cm, mole, sec, K, and cal/mole, respectively. Note that  $T$  is always in Kelvin. ANSYS Chemkin-Pro uses the thermal calorie, 4.184 Joules.

**Table 3.4: Alphabetical Listing of REACTIONS-line Options for Gas-phase Kinetics Data**

Keyword	Definition
CAL/[MOLE]	Reiterates the default units for all gas-phase reactions that follow the REACTIONS header line for parameters with energy units such as $E_i$ .  <b>Notes</b> - Default units for $E_i$ are cal/mole.
EVOL[TS]	Supersedes the default units for all gas-phase reactions which follow the REACTIONS header line for parameters with energy units such as $E_i$ .  <b>Notes</b> - Default units for $E_i$ are cal/mole.
JOUL[ES/MOLE]	Supersedes the default units for all gas-phase reactions which follow the REACTIONS header line for parameters with energy units such as $E_i$ .  <b>Notes</b> - Default units for $E_i$ are cal/mole.



Keyword	Definition
KCAL[/MOLE]	Supersedes the default units for all gas-phase reactions which follow the REACTIONS header line for parameters with energy units such as $E_i$ .  <b>Notes</b> - Default units for $E_i$ are cal/mole.
KELV[INS]	Supersedes the default units for all gas-phase reactions which follow the REACTIONS header line for parameters with energy units such as $E_i$ .  <b>Notes</b> - Default units for $E_i$ are cal/mole.
KJOU[LES/MOLE]	Supersedes the default units for all gas-phase reactions which follow the REACTIONS header line for parameters with energy units such as $E_i$ .  <b>Notes</b> - Default units for $E_i$ are cal/mole.
MOLEC[ULES]	Supersedes the default units for all gas-phase reactions which follow the REACTIONS header line for pre-exponential factors $A_i$ .  <b>Notes</b> - Default units for $A_i$ are cgs (cm, sec, K, mole), the exact units depending on the order of the reaction.
MAXSP	Increases the maximum number of reactants or products allowed in a reaction. The number given by this keyword must be greater than the default limit of 6. For example, REACTIONS MAXSP=11.  <b>Notes</b> -This keyword is available to both the gas-phase and surface reaction mechanism.
MOLE[S]	Supersedes the default units for all gas-phase reactions which follow the REACTIONS header line for pre-exponential factors $A_i$ .  <b>Notes</b> - Default units for $A_i$ are cgs (cm, sec, K, mole), the exact units depending on the order of the reaction.
USRPROD	Indicates that the user will provide a user-written rate routine that will supply all of the species net rates of production, overriding any other reaction input in the <i>Gas-phase Kinetics</i> input file.  The net rate-of-production for all species will be obtained by calling the user-supplied subroutine, CKUPROD. An optional slash(/)-delimited integer parameter allows the user to select from more than one type of rate formulation. Wherever the species production rates are required, they will be obtained by calling the user-written subroutine called CKUPROD. A template of CKUPROD is provided in the ANSYS Chemkin-Pro installation, in the file <i>cklib_user_routines.f</i> located in the directory <i>user_subroutines</i> . Information about how to compile and link user routines into Chemkin-Pro is included in <a href="#">Chemkin-Pro Application Programming Interface Manual</a> .



Keyword	Definition
	<b>Notes</b> - USRPROD cannot be used in conjunction with <a href="#">USRPROG</a> (entered after a particular reaction).

**Note:**

This API does not support user-written programming, so you are cautioned to use the CKUPROD user-routine feature at your own risk. Also, there are some features in ANSYS Chemkin-Pro that will be incompatible with the global replacement of species rates of production, such as sensitivity analysis and rate-of-production analysis. Such features will return zero values when user-rate programming is encountered.

### 3.6.2. Reaction Data

Reaction Data follows the REACTIONS line and precedes an END statement that concludes the Reactions Data section. Each reaction entry line is divided into two fields. The first contains the symbolic description of the reaction path for that reaction while the second contains the Arrhenius rate coefficients. Both fields are format-free and blank spaces are ignored. Any line or portion of a line starting with an exclamation mark (!) is considered a comment and is ignored. Blank lines are also ignored.

The reaction description, given in the first field, must be composed of the species symbols, coefficients, delimiters, and any special symbols defined in [Table 3.5: Reaction Data Criteria \(p. 41\)](#).

**Table 3.5: Reaction Data Criteria**

Species Symbols	
	Each species in a reaction is described with the unique sequence of characters as they appear in the species data and the thermodynamic data (e.g., H <sub>2</sub> ).
Coefficients	
	A species symbol may be preceded by an integer or real coefficient. The coefficient has the meaning that there are that number of moles of the particular species present as either reactants or products; e.g. 2OH, is equivalent to OH + OH. Non-integer coefficients are allowed in <i>Gas-phase Kinetics input</i> , but the element balance in the reaction must still be maintained.
Delimiters	
+	A plus sign is the delimiter between each reactant species and each product species.
=	An equality sign is the delimiter between the last reactant and the first product in a reversible reaction.
<=>	An equality sign enclosed by angle brackets can also be used as the delimiter between the last reactant and the first product in a reversible reaction.
=>	An equality sign with an angle bracket on the right is the delimiter between the last reactant and the first product in an irreversible reaction.
Special Symbols	
+M	An M as a reactant and product stands for an arbitrary third body. An M in the reaction description indicates that a third body is participating in the reaction. In a reaction containing an M, species can be specified to have enhanced third body efficiencies, in which case auxiliary information (described below) must

Species Symbols	
	follow the reaction line. If no enhanced third body efficiencies are specified, then all species act equally as third bodies and the effective concentration of the third body is the total concentration of the mixture.
(+M)	An M as a reactant and product surrounded by parentheses indicates that the reaction is a pressure-dependent reaction, in which case auxiliary information line(s) (described below) must follow the reaction to identify the fall-off formulation and parameters. A species may also be enclosed in parenthesis. Here, for example, (+H <sub>2</sub> O) indicates that water is acting as the third body in the fall-off region, not the total concentration M.
E	The symbol E as a reactant and/or product is used to represent an electron. An electron is treated just like any other species, and is composed of the element E, which must be declared as element data. If an E appears in any reaction, then it must also be declared as a species in the species data.
!	An exclamation mark means that all following characters are comments on the reaction. For example, the comment may be used to give a reference to the source of the reaction and rate data.

The second field of the REACTIONS line is used to define the Arrhenius rate coefficients  $A_i$ ,  $\beta_i$ , and  $E_i$ , in that order, as given by Equation 3.5 of the [Chemkin-Pro Theory Manual](#). At least one blank space must separate the first number and the last symbol in the reaction. The three numbers must be separated by at least one blank space, be stated in either integer, floating point, or "E" format (e.g., 123, 123.0 or 123E1), and have units associated with them.

### Note:

Unless modified by options specified on the REACTIONS line or in Auxiliary Reaction Keywords, the default units for  $A_i$  are in cgs (cm, sec, K, mole), the exact units depending on the reaction. The factor  $\beta_i$  is dimensionless. The default units for the activation energies are cal/mole.

Examples of reaction data are shown in [Figure 3.4: Examples of Reaction Data \(p. 42\)](#).

**Figure 3.4: Examples of Reaction Data**

```

REACTIONS                                CAL/MOLE    ! these are the default units for the reaction rates
H2 + O2 = 2OH                            1.7E13 0 47780. ! Ref. 21
! H2 + O2 = OH + H                      1.7E13 0 47780. ! same as previous reaction,
                                           ! commented to prevent a duplication error
H + O2 + M = HO2 + M                    2.0E15 0.000 -870.
! H + O2 + M = HO2                      2.0E15 0.000 -870.
! H + O2 = HO2 + M                      2.0E15 0.000 -870.
OH+ + H + E = H2O                        1.E19 0 0.0
O = O(*)                                1.3E5 0 0
                                           ! photoactive reaction, represented without HV
0.5H2 + 0.5O2 = OH                      ! example of real coefficients
END                                       ! END statement is optional; ! <eof> condition is equivalent

```

Table 3.6: Summary of the Rules for Reaction Data (p. 43) is a summary of the reaction data rules.

**Table 3.6: Summary of the Rules for Reaction Data**

Rule	Description
1	The first reaction line must start with the word REACTIONS (or REAC), and may include units definition(s).
2	The reaction description can begin anywhere on the line. All blank spaces, except those between Arrhenius coefficients, are ignored.
3	Each reaction description must have =, <=> or => between the last reactant and the first product.
4	Each reaction description must be contained on one line.
5	Three Arrhenius coefficients must appear in order ( $A_i$ , $\beta_i$ , and $E_i$ ) on each Reaction line, separated from each other and from the reaction description by at least one blank space; no blanks are allowed within the numbers themselves.
6	There cannot be more than six reactants or six products in a reaction.
7	Comments are any and all characters following an exclamation mark.
8	For best results an END statement should follow the reaction input.

### 3.6.3. Auxiliary Reaction Data

Auxiliary Reaction Data is entered in lines immediately following the Reaction Data for a specific reaction path. The format of an auxiliary information line is a character-string keyword followed by a slash-delimited (/) field, which begins and ends with a slash (/), and which contains an appropriate number of parameters (either integer, floating point, or "E" format).

These data or keywords are used to indicate different reaction-rate expressions, units, pressure-dependency, and other ways in which the reaction behavior may be modified. Table 3.8: Summary of the Rules for Auxiliary Reaction Data (p. 57) provides detailed information about the meaning and usage of each auxiliary keyword entry option for gas-phase reactions. Also, Figure 3.5: Examples of Auxiliary Reaction Data (p. 56) provides some additional examples of reaction data.

**Table 3.7: Alphabetical Listing of Gas-phase Reaction Auxiliary Keywords**

Keyword	Definition			
<SpeciesName>	<b>Neutral Third Body Efficiency</b> - If a reaction contains $M$ as a reactant and/or product, auxiliary information lines may follow the reaction line to specify enhanced third-body efficiencies of certain species (i.e., $a_{kir}$ , Equation 3.19 of the <a href="#">Chemkin-Pro Theory Manual</a> ). To define an enhanced third body efficiency, the keyword is the species name of the third body, and its one parameter is its enhanced efficiency factor. A species that acts as an enhanced third body must be declared as a species. Examples of third body efficiencies are shown in the first three reactions in <a href="#">Figure 3.5: Examples of Auxiliary Reaction Data (p. 56)</a> .			
	Parameters	Optional/Reqd.	Units	Examples
	Species name	Required	--	CO/1.87/

Keyword	Definition			
	<i>Stoichiometric coefficient <math>\nu_{ki}</math></i>	Required	--	CO/1.87/
	<b>Reaction Example</b>	REACTIONS CAL/MOLE HCO+M=H+CO+M 0.250E+15 0.000 16802.000 ! Warnatz CO/1.87/ H2/1.87 CH4/2.81/ CO2/3./ H2O/5./		
CHEB	<b>Chebyshev Polynomial Rate Expressions</b> - Supersedes the default reaction rate expression by a Chebyshev polynomial evaluation (see <a href="#">Equation 3.43</a> of the <a href="#">Chemkin-Pro Theory Manual</a> ). CHEB must be followed by (slash delimited) parameters; for the first CHEB, the first value is $N$ , the number of basis functions along the temperature axis; the second is $M$ , the number of basis functions along the pressure axis; and the remainder are the $N \times M$ coefficients $a_{nm}$ from <a href="#">Equation 3.41</a> in the order of $a_{11}, a_{12}, \dots, a_{1M}, a_{21}, a_{22}, \dots, a_{NM}$ , in this or additional CHEB declarations.			
	Parameters	Optional/Reqd.	Units	Examples
	Number of temperature functions $N$	Required	--	CHEB / 7 3 -4.1624 .9394 -.18563 12.438/
	Number of pressure functions $M$	Required	--	CHEB / 7 3 -4.1624 .9394 -.18563 12.438/
	Chebyshev coefficients $a$	Required	--	CHEB / 7 3 -4.1624 .9394 -.18563 12.438/
	<b>Reaction Example</b>	C2H5 + O2 (+M) <=> C2H4E + HO2 (+M) 1.00E+00 .000 0. ! mecon 7/97  CHEB/ 7 3 1.0216E+01 - 1.1083E+00 -1.9807E-01 7.8325E-01/  CHEB/ 1.1609E+00 1.1762E-01 - 9.5707E-02 1.0928E-01 1.1551E-01/  CHEB/ -8.0290E-02 -1.0978E-01 3.7074E-04 -1.4830E-02 -6.0589E-02/  CHEB/ -2.8056E-02 6.9203E-03 - 9.7259E-03 -1.3556E-02 7.6648E-03/  CHEB/ 6.6865E-03 -8.8244E-04/		
	<b>Notes</b>	<ul style="list-style-type: none"><li>More than one set of CHEB data can appear for a given reaction, as many as required to input exactly <math>N \times M + 2</math> values.</li></ul>		

Keyword	Definition	
		<ul style="list-style-type: none"> <li>Pressure limits of the Chebyshev polynomial for this reaction may be provided by keyword <a href="#">PCHEB</a> .</li> <li>Temperature limits of the Chebyshev polynomial for this reaction may be provided by keyword <a href="#">TCHEB</a> .</li> </ul>
COLLEFF	<p><b>Efficiency of Collision Frequency Expression</b> - If a reaction is bimolecular and the approximate collision diameters are known, then the collision frequency efficiency expression can be used to calculate the reaction rate constant.</p> <p>The Arrhenius parameters for the correction factor are specified on the reaction line. On the line following, the keyword COLLEFF is required to tell the interpreter the type of reaction.</p> <p>A+B&lt;=&gt;Products a b c</p> <p>COLLEFF</p> <p>In addition to the parameters for the correction factor <i>a</i>, <i>b</i>, and <i>c</i>, the diameters for each reacting species must be specified. ANSYS Chemkin-Pro uses the Lennard-Jones diameter as an approximation for the spherical diameter of a species. The Lennard-Jones diameter is one of the inputs read by the <i>Transport Pre-Processor</i> that are specified as outlined in <a href="#">Transport Data Format (p. 87)</a> .</p>	
	<b>Reaction Example</b>	<pre>C6H6 + C6H6 =&gt; C12H10 + H2 0.02 0 0 COLLEFF</pre>
DUP	<p><b>Duplicate Reactions</b> - Two or more reactions can involve the same set of reactants and products, but proceed through distinctly different processes. In these cases, it may be appropriate to state a reaction mechanism that has two or more reactions that are the same, but have different rate parameters. However, duplicate reactions are normally considered errors by the <i>Gas-phase Kinetics Pre-Processor</i>. If the user requires duplication (e.g., the same reactants and products with different Arrhenius parameters), the keyword DUP must follow the reaction line of each duplicate reaction, including the first occurrence of the reaction that is duplicated. For example, if the user wishes to specify different rate expressions for each of two identical reactions, there must be two occurrences of the DUP keyword, one following each of the reactions. No auxiliary parameters are required. Examples are shown in <a href="#">Figure 3.5: Examples of Auxiliary Reaction Data (p. 56)</a> .</p>	
	<b>Reaction Example</b>	<pre>HO2+HO2=H2O2+O2 4.20E14 0.0 11982 DUP HO2+HO2=H2O2+O2 1.3E11 0.0 -1629</pre>

Keyword	Definition			
		DUP		
EXCI	<b>Energy Loss Parameter</b> - Auxiliary data may be used to specify the energy loss per reaction event by specifying the keyword EXCI, followed by the value of the energy loss per event, in units of electron volts. This option overrides the calculation of energy loss from the change in enthalpy determined by the reaction description and the thermodynamic data of the reactants and products. The option is useful in describing electron-impact excitation reactions, for example, where the user does not wish to keep track of the excited-species density, but wants to include the energy loss to the electrons due to the excitation process. An example of the use of EXCI is given in <a href="#">Figure 3.5: Examples of Auxiliary Reaction Data (p. 56)</a> . The EXCI keyword represents the $\Delta H_r$ parameter that is used to describe inelastic collisions in <a href="#">Equation 8.128</a> of the <a href="#">Chemkin-Pro Theory Manual</a> for the electron balance in plasma simulations.			
	Parameters	Optional/Reqd.	Units	Examples
	Energy loss per event	Required	electron-volts	TDEP/E/ EXCI/11.60/
	Reaction Example	E + AR => AR + E 2.235E16 0.0 3.47E5  TDEP/E/ EXCI/11.60/  DUP		
FIT1	Supersedes the default reaction rate expression by the reaction rate described by <a href="#">Equation 3.50</a> of the <a href="#">Chemkin-Pro Theory Manual</a> . FIT1 must be followed by the four slash-delimited FIT1 parameters, <i>bni</i> .			
	Parameters	Optional/Reqd.	Units	Examples
	FIT1 parameters $b_1 - b_4$	Required	--	FIT1/33756 -1.695E8 1.08E13 0.0/
	Reaction Example	E + O2 => O + O- 4.60E-11 0.0 0.  TDEP/E/  FIT1/33756 -1.695E8 1.08E13 0.0/		
FORD	<b>Forward Reaction Order Parameter</b> - Supersedes the forward reaction order for any species in the mechanism (with respect to species concentration), regardless of whether the species appears as a reactant or a product in the reaction. FORD is followed, in slash-delimited format, by the species name and the new reaction order. This option overrides the values of $\nu_{ki}$ in <a href="#">Equation 3.4</a> of the <a href="#">Chemkin-Pro Theory Manual</a> pertaining to the particular species named on the line. The reaction order for all other species maintain their default values.			
	Parameters	Optional/Reqd.	Units	Examples
	Species name	Required	--	FORD /Pt(S) 1.0/

Keyword	Definition			
	<i>Stoichiometric coefficient <math>\nu_{ki}</math></i>	Required	--	FORD /Pt(S) 1.0/
	<b>Reaction Example</b>	JP10+14O2 => 10CO2 + 8H2O 6.454323E+13 0.0 29188.8  FORD / JP10 1.153923 /  FORD / O2 0.738210 /		
	<b>Notes</b>	Multiple occurrences of the FORD construct may appear on the auxiliary line.		
HIGH	Defines the high-pressure limit for pressure-dependent chemically activated bimolecular reactions (see Equation 3.26 of the Chemkin-Pro Theory Manual ). HIGH must be followed by the three slash-delimited high-pressure limit Arrhenius parameters $A_\infty$ , $\beta_\infty$ , and $E_\infty$ , and the Arrhenius coefficients on the reaction line represent the low-pressure limit Arrhenius parameters $A_0$ , $\beta_0$ , and $E_0$ .			
	Parameters	Optional/Reqd.	Units	Examples
	Pre-exponential factor $A_\infty$	Required	Depends on reaction	HIGH /6.85E-12 6.53 -834./
	Temperature exponent $\beta_\infty$	Required	--	HIGH /6.85E-12 6.53 -834./
	Activation energy $E_\infty$	Required	cal/mole	HIGH /6.85E-12 6.53 -834./
	<b>Reaction Example</b>	C2H5+O2 (+M)= C2H4+HO2 (+M) 1.41E7 1.09 -1975.  HIGH/6.85E-12 6.53 -834./  TROE/0.45 1.E-10 1.E10/  H2/2/ CO/2/ CO2/3/ H2O/5/		
	<b>Notes</b>	<ul style="list-style-type: none"><li>Required when SRI or TROE is present</li><li>Additional pressure-dependency parameters may be provided by keywords SRI or TROE.</li><li>If no additional parameters, the Lindemann formulation is applied.</li></ul>		
JAN	<b>Optional Rate Fit Expressions</b> - Supersedes the default reaction rate expression by a Janev-Langer reaction rate (see Equation 3.49 of the			

Keyword	Definition			
	Chemkin-Pro Theory Manual ). JAN must be followed by the nine slash-delimited Janev-Langer rate parameters, $b_{ni}$ .			
	Parameters	Optional/Reqd.	Units	Examples
	Janev-Langer parameters $b_1$ - $b_9$	Required	eV	JAN / -19.73476 3.992702 -1.773436 0.5331949 -0.1 0.02 -0.002 8.E-5 -2.E-6/
	Reaction Example	$H^* + E = H + 2E$ 1.0 0.0 0.0  JAN / -19.73476 3.992702 -1.773436 0.5331949 -0.1 0.02 -0.002 8.E-5 - 2.E-6/		
	Notes	<ul style="list-style-type: none"><li>If fewer than 9 parameters are required for the fit, the user must provide zeros for the remainder of the parameters.</li><li>The Janev rate expression was originally designed for usage with plasmas, and the temperature unit is eV (i.e., electron-volt). When the rate is calculated, the system temperature is first converted to eV. For temperatures in kelvin, it will be <math>T/11595</math> in eV. Therefore the temperature needs to be in eV when fitting the JAN rate coefficients, while other reactions in the mechanism still use temperature in K.</li></ul>		
LOW	Defines the low-pressure limit for pressure-dependent unimolecular fall-off reactions (see Equation 3.25 of the Chemkin-Pro Theory Manual ). LOW must be followed by the slash-delimited low-pressure limit Arrhenius parameters $A_o$ , $\beta_o$ , and $E_o$ , and the Arrhenius coefficients on the reaction line represent the three high-pressure limit Arrhenius parameters $A_\infty$ , $\beta_\infty$ , and $E_\infty$ .			
	Parameters	Optional/Reqd.	Units	Examples
	Pre-exponential factor $A_o$	Required	depends on reaction	LOW /1.73E69 -15.07 60491./
	Temperature exponent $\beta_o$	Required	--	LOW /1.73E69 -15.07 60491./
	Activation energy $E_o$	Required	cal/mole	LOW /1.73E69 -15.07 60491./
	Reaction Example	$O + CO (+M) \rightleftharpoons CO_2 (+M)$ 1.800E+10 .000 2385.00  LOW/ 6.020E+14 .000 3000.00/		
	Notes	<ul style="list-style-type: none"><li>Required when SRI or TROE is present</li><li>Supplemental pressure-dependency parameters may be provided by keywords SRI or TROE.</li></ul>		



Keyword	Definition			
		• If no additional parameters, the Lindemann formulation is applied.		
LT	<b>Landau-Teller Reactions</b> - Supersedes the default reaction rate expression by the Landau-Teller reaction rate (see <a href="#">Equation 3.47</a> of the <a href="#">Chemkin-Pro Theory Manual</a> ). LT must be followed by the two slash-delimited Landau-Teller reaction rate parameters <i>Bi</i> and <i>Ci</i> .			
	Parameters	Optional/Reqd.	Units	Examples
	Landau-Teller parameter <i>B<sub>i</sub></i>	Required	--	LT /-67 62.1/
	Landau-Teller parameter <i>C<sub>i</sub></i>	Required	--	LT /-67 62.1/
	Reaction Example	H2 ( 1 ) +H2O ( 000 ) =H2 ( 0 ) +H2O ( 001 ) 2.89E15    0    0  LT   /   -67    62.1/		
	Notes	If explicit <a href="#">REV</a> parameters are given for the reaction, then explicit reverse Landau-Teller parameters must also be given by keyword <a href="#">RLT</a> .		
MOME	<b>Plasma Momentum-Transfer Collision Frequency Options</b> - Indicates that the reaction parameters describe the momentum-transfer collision frequency for electrons. This keyword requires no supplemental data, but changes the treatment of the reaction-rate coefficients. The option causes the reaction to be flagged as an electron momentum-transfer reaction, and assumes that the reaction rate constant is in units of cm <sup>3</sup> /mole-s or cm <sup>3</sup> /molecule-s, depending on the units specified in the REACTIONS statement. These reactions are treated as special cases when <i>Gas-phase Kinetics</i> subroutines evaluate reaction rates-of-progress, as described in <a href="#">Rates of Creation and Destruction of Species</a> of the <a href="#">Chemkin-Pro Theory Manual</a> .			
	Reaction Example	E + AR* => E + AR* 1.0502E-08 2.5929E-01 1.7464E+04  TDEP /E/  MOME		
	Notes	These options would generally not be used (or would be ignored) with any of the standard ANSYS Chemkin-Pro reactor models; they are there for users who may be incorporating Chemkin-Pro into a multi-dimensional plasma simulation user program.		
PCHEB	Supersedes the default pressure limits for a Chebyshev polynomial rate expression (see <a href="#">Equation 3.42</a> of the <a href="#">Chemkin-Pro Theory Manual</a> ). PCHEB must be followed by the two slash-delimited values <i>Pmin</i> and <i>Pmax</i> .			
	Parameters	Optional/Reqd.	Units	Examples

Keyword	Definition			
	Minimum pressure $P_{min}$	Required	atm	PCHEB / 1.0 100.0/
	Maximum pressure $P_{max}$	Required	atm	PCHEB / 1.0 100.0/
	Reaction Example	C2H5+O2 (+M)=C2H4E+HO2 (+M) 1.0 0.0 0.0  LOW / 1.0 0.0 0.0 /  PCHEB / 1.0 100.0/  CHEB/ 7 3 10.216 -1.1083 -0.19807 0.78325/  CHEB/ 1.1609 0.1.1762 -0.095707 0.10928 0.11551/  CHEB/ -0.08029 -0.10978 3.7074E-04 -0.01483 -0.060589/  CHEB/ -0.028056 6.9203E-03 - 9.7259E-03 -0.013556 7.6648E-03/  CHEB/ 6.6865E-03 -8.8244E-04/		
	Notes	<ul style="list-style-type: none"><li>The default Chebyshev polynomial pressure limits are <math>P_{min}=0.001</math>, <math>P_{max}=100</math>.</li><li>Chebyshev polynomial parameters must be provided by use of keyword <a href="#">CHEB</a>.</li><li>Default Chebyshev polynomial temperature limits may be superseded by keyword <a href="#">TCHEB</a>.</li></ul>		
PLOG	<b>Pressure Dependence Through Logarithmic Interpolation</b> - Provides a general-purpose way of describing pressure-dependent reaction rates. Using the PLOG keywords, you can enter any number of sets of Arrhenius reaction-rate coefficients at different reactor pressures. The PLOG data will override the Arrhenius coefficients provided on the reaction line. The PLOG keyword must be followed by the slash-delimited values for the pressure at which the reaction rates are given and the three Arrhenius parameters, $A_i$ , $\beta_i$ , and $E_i$ , for that pressure. Multiple PLOG entries can be provided, but they must be included in ascending order of pressure. See the ANSYS Chemkin-Pro Theory Manual, <a href="#">General Pressure Dependence Using Logarithmic Interpolation</a> , <a href="#">General Pressure Dependence Using Logarithmic Interpolation</a> .			
	Parameters	Optional/Reqd.	Units	Examples
	Pressure		atm	PLOG /0.03947 2.9512E+09 1.28 13474./

Keyword	Definition			
	Pre-exponential factor $A_i$		Depends on reaction	PLOG /0.03947 2.9512E+09 1.28 13474./
	Temperature exponent $\beta_i$		--	PLOG /0.03947 2.9512E+09 1.28 13474./
	Activation energy $E_i$		cal/mole	PLOG /0.03947 2.9512E+09 1.28 13474./
	Reaction Example	H2CCCH+H=C3H2 ( S ) +H2                    2.9512E+09 		

Keyword	Definition			
		REV / 9.381E-14 0. 31404.1 /		
RLT	Supersedes the default reverse reaction rate expression by the Landau-Teller reaction rate (see Equation 3.47 of the Chemkin-Pro Theory Manual ). RLT must be followed by the two slash-delimited Landau-Teller reaction rate parameters $B_i$ and $C_i$ .			
	Parameters	Optional/Reqd.	Units	Examples
	Landau-Teller parameter $B_i$	Required	--	RLT /-67 62.1/
	Landau-Teller parameter $C_i$	Required	--	RLT /-67 62.1/
	Reaction Example	H2 ( 1 ) +H2O ( 000 ) =H2 ( 0 ) +H2O ( 001 ) 2.89E15 0 0  RLT / -67 62.1/		
	Notes	<ul style="list-style-type: none"><li>Required when the combination of LT and REV keywords is present.</li><li>If explicit REV parameters are given for the reaction, then explicit reverse Landau-Teller parameters must also be given by keyword RLT.</li></ul>		
RORD	<b>Reverse Reaction Order Parameter</b> - Supersedes the reverse reaction order for any species in the mechanism (with respect to species concentration), regardless of whether the species appears as a reactant or a product in the reaction. RORD must be followed by the slash-delimited species name and the new reaction order, and supersedes the values of $\nu''_{ki}$ in Equation 3.4 of the Chemkin-Pro Theory Manual pertaining to the particular species named on the line; the reaction order for all other species maintain their default values. Multiple occurrences of the RORD construct may appear on the auxiliary line.			
	Parameters	Optional/Reqd.	Units	Examples
	Species name	Required	--	RORD /OH 2.0/
	Stoichiometric coefficient $\nu''_{ki}$	Required	--	RORD /OH 2.0/
	Reaction Example	H2+O2=2OH 0.170E+14 0.00 47780  RORD /OH 2.0/		
	Notes	See also FORD.		
SRI	Defines the SRI pressure-dependent reaction rate (see Equation 3.34 of the Chemkin-Pro Theory Manual ). SRI must be followed by either three, or five, slash-delimited parameters $a$ , $b$ , $c$ , $d$ , and $e$ . The fourth and fifth parameters are optional and if omitted, they are by default $d = 1$ and $e = 0$ .			
	Parameters	Optional/Reqd.	Units	Examples

Keyword	Definition			
	<i>SRI reaction rate parameters a - e</i>	Required	--	SRI /0.45 797. 979. 1.0 0.0/
	<b>Reaction Example</b>	CH3+H(+M) = CH4(+M) 6.0E16 -1.0 0  LOW/8.0E26 -3.0 0/  SRI/0.45 797.0 979.0/  H2/2/ CO/2/ CO2/3/ H2O/5/		
	<b>Notes</b>	• Additional SRI parameters are required, by use of keywords <a href="#">LOW</a> or <a href="#">HIGH</a> .		
TCHEB	Supersedes the default temperature limits for a Chebyshev polynomial rate expression (see <a href="#">Equation 3.41</a> of the <a href="#">Chemkin-Pro Theory Manual</a> ). TCHEB must be followed by the slash-delimited values, <i>Tmin</i> and <i>Tmax</i> .			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Minimum temperature Tmin</i>	Required	K	TCHEB / 300.0 2500./
	<i>Maximum temperature Tmax</i>	Required	K	TCHEB / 300.0 2500./
	<b>Reaction Example</b>	C2H5+O2(+M)=C2H4E+HO2 (+M) 1.0 0.0 0.0  LOW / 1.0 0.0 0.0 /  TCHEB / 300. 2500./  CHEB/ 7 3 10.216 -1.1083 -0.19807 0.78325/  CHEB/ 1.1609 0.1.1762 -0.095707 0.10928 0.11551/  CHEB/ -0.08029 -0.10978 3.7074E-04 -0.01483 -0.060589/  CHEB/ -0.028056 6.9203E-03 -9.7259E-03 -0.013556 7.6648E-03/  CHEB/ 6.6865E-03 -8.8244E-04/		
	<b>Notes</b>	• The default Chebyshev polynomial temperature limits are <i>Tmin</i> =300, <i>Tmax</i> =2500.  • Required Chebyshev polynomial parameters must be provided by use of keyword <a href="#">CHEB</a> .		

Keyword	Definition			
		<ul style="list-style-type: none"><li>Supplemental Chebyshev polynomial pressure limits may be provided by use of keyword <b>PCHEB</b>.</li></ul>		
TDEP	<b>Species Temperature Dependence</b> - Causes the reaction rate constant to be evaluated using the specified species temperature and the rate parameters given in the reaction data. In the case when there is more than one temperature defined in the system, the Application must call the <i>Gas-phase Kinetics</i> subroutine <b>CKKTFL</b> to indicate which temperature in the temperature array corresponds to each species. Examples of the <b>TDEP</b> input are shown in <a href="#">Figure 3.5: Examples of Auxiliary Reaction Data (p. 56)</a> .			
	Parameters	Optional/Reqd.	Units	Examples
	Species name	Required	--	TDEP/E/
	Keyword Usage	E + CL2 => CL- + CL 5.8901E-09 - 2.5619E-01 1.5834E+04  TDEP/E/		
TROE	Defines the Troe pressure-dependent reaction rate (see <a href="#">Equation 3.33</a> of the <a href="#">Chemkin-Pro Theory Manual</a> ). <b>TROE</b> must be followed by the slash-delimited 3 or 4 parameters $\alpha$ , $T^{***}$ , $T^*$ , and $T^{**}$ ; the fourth parameter is optional and if omitted, the last term in <a href="#">Equation 3.33</a> is not used.			
	Parameters	Optional/Reqd.	Units	Examples
	$\alpha$	Required	Depends on reaction	TROE /0.5336 629.2 2190.626.5/
	$T^{***}$	Required	K	TROE /0.5336 629.2 2190.626.5/
	$T^*$	Required	K	TROE /0.5336 629.2 2190.626.5/
	$T^{**}$	Optional	K	TROE /0.5336 629.2 2190.626.5/
	Reaction Example	C2H5+O2(+M)= C2H4+HO2(+M) 1.41E7 1.09 -1975.  HIGH/6.85E-12 6.53 -834./  TROE/0.45 1.E-10 1.E10/  H2/2/ CO/2/ CO2/3/ H2O/5/		
	Notes	Other required <b>TROE</b> parameters must be provided by use of keywords <b>LOW</b> or <b>HIGH</b> .		
UNITS	<b>Reaction Units</b> - Supersedes the current units for a particular reaction rate fit that may differ from the default units specified for other reaction expressions in the chemistry mechanism. <b>UNITS</b> must be followed by the slash-delimited character-string <b>string</b> , where <b>string</b> is one of the following: <b>EVOL[ TS ]</b> , <b>KELV[ INS ]</b> , <b>CAL/[ MOLE ]</b> , <b>KCAL[ /MOLE ]</b> , <b>JOUL[ ES/MOLE ]</b> , or <b>KJOUL[ LES/MOLE ]</b> for parameters with energy units such as $E_i$ or			

Keyword	Definition			
	MOLES or MOLEC[ULES] for pre-exponential factors $A_i$ , where the letters in brackets are optional. The inclusion of MOLEC[ULES] would indicate that the reaction rate expression is in units of molecules/cm <sup>3</sup> rather than mole/cm <sup>3</sup> . The UNITS auxiliary keyword allows only one string parameter, but the user can repeat the UNITS as many times as needed for a given reaction.			
	Parameters	Optional/Reqd.	Units	Examples
	Reaction units character string	Required	--	UNITS /MOLECULES/
	Reaction Example	CF3+ + E + #WSIO2(B) => #SIO2 + CF3 0.33 0.0 0.0  BOHM !  YIELD /0.01 20. 0.5 1.0/ UNITS/EVOLTS/		
	Notes	<ul style="list-style-type: none"><li>• Default units for <math>A_i</math> are cgs (cm, sec, K, mole), the exact units depending on the order of the reaction.</li><li>• Default units for <math>E_i</math> are (cal/mole).</li><li>• If any of the units strings are given on the REACTIONS header line, it applies to all reactions, but may be superseded for a particular reaction by the auxiliary UNITS keyword</li><li>• Even if the default energy units are changed by giving the UNITS keyword, the temperature appearing in the Arrhenius expression of <a href="#">Equation 3.5</a> of the <a href="#">Chemkin-Pro Theory Manual</a> is still in Kelvins.</li></ul>		
USRPROG	<b>Optional User Rate Subroutine CKUPROG</b> – The net rate-of-progress for the reaction will be obtained by calling a user-supplied subroutine, CKUPROG. An optional slash(/)-delimited integer parameter allows the user to select from more than one type of rate formulation. Wherever the net reaction rate is required, it will be obtained by calling the user-written subroutine. A template of CKUPROG is provided in the ANSYS Chemkin-Pro installation, in the file <b>cklib_user_routines.f</b> located in the directory <b>user_routines</b> . Information about how to compile and link user routines into Chemkin-Pro is included in <a href="#">Chemkin-Pro Application Programming Interface Manual</a> .			
	Parameters	Optional/Reqd.	Units	Examples
	Rate formulation type	Optional	--	USRPROG /1/
	Reaction Example	H2+O2=>2OH 47780.  USRPROG /1 /		

Keyword	Definition	
	Notes	<ul style="list-style-type: none"> <li>USRPROG applies only to irreversible reactions, and cannot be used in conjunction with USRPROD (entered on the REACTIONS header line).</li> </ul>
XSMI	<p>Flags a reaction as representing collision cross-section information for the determination of ion momentum-transfer collision frequencies in a plasma simulation. No auxiliary parameters are required. The evaluated rate-constant is assumed to be in <math>\text{cm}^2</math>, and is left as such when <i>Gas-phase Kinetics</i> subroutines evaluate rates of progress for other reactions. For more detail, see <a href="#">Rates of Creation and Destruction of Species</a> of the <i>Chemkin-Pro Theory Manual</i>. Examples are given in <a href="#">Figure 3.5: Examples of Auxiliary Reaction Data</a> (p. 56).</p>	
	Reaction Example	<pre>CL+ + CL =&gt; CL+ + CL 1.03E-13 -0.5 0.0  TDEP/CL+/  XSMI      !momentum-transfer x-sec</pre>
	Notes	<ul style="list-style-type: none"> <li>These options would generally not be used (or would be ignored) with any of the standard ANSYS Chemkin-Pro reactor models; they are there for users who may be incorporating Chemkin-Pro into a multi-dimensional plasma simulation user program.</li> </ul>

**Figure 3.5: Examples of Auxiliary Reaction Data**

```
REACTIONS          CAL/MOLE      ! these are the default units for the reaction rates
HCO+M=H+CO+M      0.250E+15  0.000  16802.000          ! Warnatz
CO/1.87/  H2/1.87  CH4/2.81/ CO2/3./  H2O/5./

H+C2H4(+M)=C2H5(+M)  0.221E+14  0.000  2066.000          ! Michael
  LOW / 6.369E27 -2.76 -54.0 /          !Lindemann fall-off reaction
  H2/2/  CO/2/  CO2/3/  H2O/5/          ! enhanced third-body efficiencies

CH3+CH3(+M)=C2H6(+M)  9.03E16 -1.18  654.
  LOW / 3.18E41 -7.03 2762 /
  TROE / 0.6041 6927. 132. /          ! TROE fall-off reaction, with 3 parameters
  H2/2/  CO/2/  CO2/3/  H2O/5/          ! enhanced third-body efficiencies

CH3+H(+M)=CH4(+M)   6.0E16 -1.0  0.0
  LOW / 8.0E26 -3.0 0.0/
  SRI / 0.45 797. 979. /          ! SRI fall-off reaction
  H2/2/  CO/2/  CO2/3/  H2O/5/          ! enhanced third-body efficiencies

CH3+CH3(+M)=H + C2H5(+M)  4.989E12 0.099  10600.0 ! Stewart
  HIGH/ 3.80E-7 4.838 7710. /          ! Chemically activated reaction
  SRI / 1.641 4334 2725 /          ! SRI pressure dependence

CH4+H=CH3+H2        1.25E14  0  1.190E4          ! Westbrook
  REV / 4.80E12  0  1.143E4 /

! The following two reactions are acceptable duplicates:

H2+O2 = 2OH          1.7E13  0  47780
  DUPLICATE
H2+O2 = 2OH          1.0E13  0  47000.
  DUPLICATE

H2(1)+H2O(000)=H2(0)+H2O(001)  2.89E15  0  0
```



```

LT / -67 62.1/                                ! Landau-Teller reaction

! The following is a Chebyshev polynomial rate description

C2H5 + O2 (+M)      <=> C2H4E + HO2 (+M)  1.00E+00      .000      0.      ! Bozzelli
TCHEB/ 300 2500/      PCHEB/1 100/
CHEB/ 7 3      1.0216E+01 -1.1083E+00 -1.9807E-01 7.8325E-01/
CHEB/ 1.1609E+00 1.1762E-01 -9.5707E-02 1.0928E-01 1.1551E-01/
CHEB/ -8.0290E-02 -1.0978E-01 3.7074E-04 -1.4830E-02 -6.0589E-02/
CHEB/ -2.8056E-02 6.9203E-03 -9.7259E-03 -1.3556E-02 7.6648E-03/
CHEB/ 6.6865E-03 -8.8244E-04/

! The following reactions allow plasma kinetics descriptions
E + E + AR+ <=> AR + E 1.414E+39 -4.500 0.00      ! Mansbach & Keck
TDEP/E/ REV/6.807E+31 -3.0 364218./      !electron temperature dependence

E + AR => AR + E      4.9E-7 0.162 8.7634E3
TDEP/E/ MOME      !Momentum-transfer collision frequency
UNITS/KELVIN/

AR+ + AR => AR+ + AR      1.E-16 0.0 0.0      !units of cm^2
XSMI      !Ion momentum-transfer collision cross-section

E + AR => AR + E      2.235E16 0.0 3.47E5
TDEP/E/ EXCI/11.60/ ! metastable excitation reaction
DUP

H2O+H = OH+H2      0.117E+10 1.30 3626
FORD /H2O 1.1/

END      !END line is optional

```

### 3.6.3.1. Problems Having No Reactions

In some problems only information about the elements and species is needed (e.g., chemical equilibrium computations). For these it is not necessary to include reaction data. The *Gas-phase Kinetics* Pre-processor will create the Linking File (e.g., *chem.asc*), but it will not contain any reaction information. Therefore, no subroutines in the *Gas-phase Kinetics* Subroutine Library that deal with chemical reactions (e.g., chemical production rates) may be used.

Table 3.8: Summary of the Rules for Auxiliary Reaction Data (p. 57) summarizes the rules for auxiliary reaction data.

**Table 3.8: Summary of the Rules for Auxiliary Reaction Data**

Rule	Description
1	Auxiliary information lines may follow reaction lines that contain an M to specify enhanced third-body efficiencies, a reversible reaction to specify the reverse rate parameters explicitly, or any reaction that specifies Landau-Teller parameters. Auxiliary information must follow any duplicate reactions as well as all reactions that indicate pressure-dependent behavior by (+M) (i.e., provide fall-off parameters).
2	A species may have only one enhanced third body efficiency associated with it in any one reaction.
3	Only one radiation wavelength may be declared in a reaction.
4	The order in which the enhanced third body declarations are given is the order in which arrays of enhanced third body information are referenced in the subroutine package.
5	There cannot be more than ten enhanced third bodies in a reaction.

Rule	Description
6	Keyword declarations may appear anywhere on the line, in any order.
7	Any number of keywords may appear on a line and more than one line may be used; however, a keyword and its parameter(s) must appear on the same line.
8	Keyword declarations that appear on the same line must be separated by at least one blank space.
9	Any blank spaces between a keyword and the first slash are ignored and any blanks between the slashes and parameter(s) are also ignored. However, no blank spaces are allowed within a keyword or a parameter.
10	All characters following an exclamation mark are comments.
11	In ion momentum-transfer collision cross-section reactions there must be exactly two reactant species, one of which must be an ion.
12	In electron momentum-transfer collision frequency reactions, there must be exactly two reactant species, one of which must be the electron.

### 3.6.4. Error Checks

The *Gas-phase Kinetics* Pre-processor checks each input line for proper syntax and writes diagnostic messages on logical file `LOUT` if errors are encountered. If an error condition occurs, the Pre-processor continues to read and diagnose the input, but an error flag is written to the Linking File and the *Gas-phase Kinetics* subroutine `CKINIT` will not initialize the work arrays. Therefore, the input must be error free before any of the *Gas-phase Kinetics* subroutines can be called. The possibilities for an error condition are listed [Table 3.9: Error Checks \(p. 58\)](#).

**Table 3.9: Error Checks**

Data Type	Possible Errors
Element Data	Atomic weight for an element or isotope is not declared, and the element is not found in the Pre-processor's database.
	Atomic weight has been declared, but not enclosed by two slashes (/).
	If an element is declared twice, a diagnostic message is printed, but the duplicate is simply eliminated from consideration and is not considered a fatal error.
Species Data	If a species is declared twice, a diagnostic message is printed, but the duplicate is eliminated from consideration and is not considered a fatal error.
	No thermodynamic data have been found for a declared species.
Thermodynamic Data	Thermodynamic data are format sensitive and therefore provide possibilities for error if not formatted exactly as described by <a href="#">Table 2.1: Summary of the Rules for Thermodynamic Data (p. 4)</a> .
	An element in the thermodynamic data for a declared species has not been included in the element data.

Data Type	Possible Errors
	With the THERMO ALL option, line 2 (Table 2.1: Summary of the Rules for Thermodynamic Data (p. 4) ) is not found.
Reaction Data	A delimiter =>, <=>, or = between the reactants and the products is not found.
	Three Arrhenius parameters are not found.
	Reactants and/or products have not been properly delineated by a plus sign (+).
	A species as a reactant or product has not been declared in the species data.
	The reaction does not balance in elements.
	The reaction does not balance in electronic charge.
	A reaction is a duplicate not declared by the auxiliary data keyword DUP.
	A third-body species enclosed in parentheses in a fall-off reaction appears as reactant or product, but not both.
	A species is a third-body in a fall-off reaction, and +M also appears in the reaction.
	More than one +M or third body appear as reactants and/or products.
	There are more than six reactants or six products.
Auxiliary Reaction Data	There is an unknown or misspelled keyword or enhanced third-body species name.
	Parameters for a keyword are not enclosed in slashes.
	The wrong number of parameters appear for a keyword.
	There are duplicate keywords for a reaction.
	LOW, HIGH, TROE, SRI, PCHEB, TCHEB, or CHEB are found after a reaction that did not have a species or M in parentheses.
	LOW, HIGH, or CHEB is not found after a pressure-dependent reaction.
	A combination of TROE, SRI, CHEB and/or PLOG is found.
	LT and REV are found for a Landau-Teller reaction, but RLT is not found.
	LT is given for a fall-off reaction.
	There are more than ten enhanced third bodies.
	There are more than or less than two reactants specified with XSMI or MOME keywords.
	An ionic species is not specified as a reactant with the XSMI keyword.
	The electron is not a reactant when using the MOME keyword.
	USRPROG given for a USRPROD mechanism.
	USRPROG given for a reversible reaction.



---

## Chapter 4: Surface Kinetics Input

---

The *Surface Kinetics* input file provides symbolic description of a surface reaction mechanism. Pre-processing this file requires obtaining information stored in the *Gas-phase Kinetics* linking file (e.g., *chem.asc*) that was created from the gas-phase mechanism associated with the chemistry set. Pre-processing the *Surface Kinetics* input file results in the creation of an additional linking file (e.g., *surf.asc*) that contains information about the surface mechanism and the species it involves. The information in the *Surface Kinetics* Linking File is subsequently accessed by the initialization routine in the *Surface Kinetics* Subroutine Library to store information in memory during a reacting-flow simulation. This stored information is then used to call other routines in the *Surface Kinetics* Subroutine Library to provide information on thermodynamic properties and chemical production rates.

The *Surface Kinetics* input includes information on surface sites (phases), surface species, bulk phases, bulk species, thermodynamic data, and the reaction mechanism. The order of data entry in the *Surface Kinetics* input file is: material name, site data, bulk data, thermodynamic data, reaction data, and a material-end statement. All input data is optional, but species included in reaction strings must be declared as site or surface species (or as gas species in the Gas Kinetics input file) and must have associated thermodynamic data included either directly in the *Surface Kinetics* input file or in a thermodynamic database file (e.g., *therm.dat*). Such sets of information can be repeated for any number of different materials within the same *Surface Kinetics* input file. With the exception of the thermodynamic data, all input is format free. The syntax and rules for all of the data input is described in this chapter. The auxiliary keywords for surface reactions are described in [Table 4.6: Alphabetical Listing of Surface Reaction Auxiliary Keywords \(p. 72\)](#) and the options for specifying units on the REACTIONS line are described in [Table 4.3: Alphabetical Listing of REACTIONS-line Options for Surface Reaction Data \(p. 66\)](#). [Alphabetical Listing of Project Input Keywords \(p. 123\)](#) describes the meaning and usage of each keyword entry that may be included as part of a Reactor Model input file.

---

### Note:

The *Surface Kinetics* Input File allows **259** columns for the presentation of the input data.

---

### 4.1. Material Declaration

---

Entirely different surface reaction mechanisms (i.e., with different surface and bulk phases and species, and different surface reactions) can be specified in the same *Surface Kinetics* input file through the use of multiple materials. At the beginning of each separate portion of the input file corresponding to a given material, the user gives an input line with the keyword MATERIAL followed by an optional space-delimited material name. If no name for the material is supplied, a default name MATERIAL **n** is provided, where **n** is the number of the material (e.g., MATERIAL2 for the second material given in an input file). An example of the usage of multiple materials is given in [Figure 4.1: Examples of Material Declarations \(p. 61\)](#).

**Figure 4.1: Examples of Material Declarations**

```
!-----GAS-PHASE KINETICS PRE-PROCESSOR INPUT-----  
ELEMENTS SI CL E AL
```

```

SPECIES      E CL2+ CL+ SICL4 SICL2 CL

NOTE THAT ABOVE IS A CHEM.INP FILE, WHILE BELOW IS A SURF.INP FILE.

!-----SURFACE KINETICS PRE-PROCESSOR INPUT-----
MATERIAL WAFER
SITE/POLY/ SDEN/2.25e-9/
SI(S)  SICL(S) SICL2(S) SICL3(S)
END
BULK SI(B)/2.33/
REACTIONS MWOFF
      CL + SI(S)      => SICL(S)                1.0   0.0   0.0
      STICK
      E + CL2+ + 2SI(S) => 2SICL(S)            0.4   0.0   0.0
      BOHM
      E + CL+ + SICL3(S) + SI(B) => SICL4 + SI(S) 0.50  0.0   0.0
      BOHM
      ENRGDEP/1. 0.5 1.0/ UNITS/EVOLT/
      E + CL+ + #SICL3(S) + #SI(B) + SICL(S) &
      => SICL2(S) + #SICL2 + #SICL(S)            0.50  0.0   0.0
      BOHM
      YIELD/0.0712 1.21 0.5 1.0/ UNITS/EVOLT/
      !          /A Eth[eV] a b / for #=A(Ei^a-Eth^a)^b
END
MATERIAL WALL
SITE/METAL/ SDEN/2.25E-9/
AL(S) ALCL(S)
END
REACTIONS MWOFF
      CL+ + E          => CL                    0.6   0.0   0.0
      BOHM
      CL + AL(S)       => ALCL(S)              1.0   0.0   0.0
      STICK
END

```

## 4.2. Site Data

Surface-phase species exist on sites, and a site and its species must be identified on one or more lines of site data. The first line in a set of site data must start with the word `SITE`; an optional name may be associated with a site if it immediately follows `SITE` and is delimited by slashes (/). If no name for the site is supplied, a default name `SITE n` is provided, where **n** is the number of a site (e.g., `SITE2` for the second site type listed). Following `SITE` and/or the site name, the word `SDEN` and a slash-delimited density (the standard state site density for this site, in mole/cm<sup>2</sup>) for the site is required. The species that can reside on the site type are declared by a list of species symbols (names) on the same line or on additional lines.

### Note:

The name of a site species must not duplicate the name of a gas-phase species or a bulk species, and must be unique among the site species for all materials.

An optional slash-delimited site occupancy number may follow a species name, i.e., the number of individual sites that this species occupies. (For example, a large chemical species might cover two or more sites.) The default site occupancy for a surface species is 1. The sets of `SITE` data input can continue for as many site types as are needed.

Any set of up to sixteen upper- or lower-case characters can be used as a site name or species symbol. In addition, each species must be composed of elements that have been identified in the *Gas-phase Kinetics* Pre-processor and thus contained in the *Gas-phase Kinetics* Linking File. One of the purposes

of the site data is to define the order in which arrays of site species information are referenced in the *Surface Kinetics* Subroutine Library.

### Note:

Species symbols may not begin with a number, a plus sign (+), a pound sign (#), or an equality sign (=), have imbedded blanks, or include a slash (/). An ionic species may end with any number of plus or minus signs; an imbedded plus sign must be enclosed in parentheses.

Any line starting with or any portion of a line following an exclamation mark (!) is considered a comment and will be ignored. Blank lines are also ignored. [Figure 4.2: Examples of Site Data \(p. 63\)](#) shows sample site data. The rules for site data are summarized in [Table 4.1: Summary of the Rules for Site Data \(p. 63\)](#).

**Figure 4.2: Examples of Site Data**

```

SITE / PLANE /          SDEN/1.04E-9/  ! PLANAR SITE
  ASH(V)                ! FIRST SPECIES ON PLANE SITE
  ASH2(V) ASH3(V) H(S) CH3(V) AS(V) AS2(V)/2/
  V                      ! EMPTY PLANAR SITE
END                      ! AN END STATEMENT IS OPTIONAL
SITE / LEDGE /          SDEN/1.66E-10/  ! LEDGE SITE
  GACH(L)               ! FIRST SPECIES ON LEDGE
  DMG(L)/2/             ! THIS SPECIES OCCUPIES 2 SITES
  L                     ! EMPTY LEDGE SITE
SITE SDEN/1.0E-10/ GA(S) ! SITE WITH ONLY ONE SPECIES
                        ! SITE NAME NOT INCLUDED

```

**Table 4.1: Summary of the Rules for Site Data**

Rule	Description
1	Site data must start with a line containing the word <code>SITE</code> , followed by an optional slash-delimited name (i.e., <code>SITE/ name /</code> ).
2	The standard state site density is required as a slash-delimited number (in mole/cm <sup>2</sup> ) following the word <code>SITE</code> and/or the site name, and preceded by the word <code>SDEN</code> .
3	The site density is followed by one or more site species name declarations. Declaring a site with no site species is an error.
4	Site and species names are composed of up to sixteen upper- or lower-case character symbols. The names cannot begin with the characters +, =, #, or a number; an ionic species name may end with one or more + or – signs; an embedded plus sign must be enclosed in parentheses ( + ). Names cannot include a slash (/).
5	All species names should be unique; duplicate species names will be ignored and a warning issued. A species name may not duplicate a name of a gas-phase species, another surface species, or a bulk species.
6	A site name must not duplicate the name of any other phase (gas, surface site, or bulk phase).
7	Each surface species that subsequently appears in a surface reaction must have been declared in this section.

Rule	Description
8	A site species name may appear anywhere on the line.
9	A site species may have a slash-delimited site occupancy (the number of sites that this species occupies on the surface) following the species name.
10	A species name declaration that begins on one line may not continue to the next line (i.e., do not break a species name into two lines).
11	There may be more than one set of <code>SITE</code> data.
12	All characters on a line following an exclamation mark are considered comments.
13	<code>SITE</code> data are not required.

### 4.3. Bulk Data

A set of bulk data may consist of one or more condensed-phase species. The first line in a set of bulk data must start with the word `BULK` and may be followed by an optional slash-delimited name for the bulk phase. If a name is not supplied for bulk phase  $n$ , then the name `BULK $n$`  is supplied. Bulk species are declared by a list of unique species symbols (names) on the same line or on additional lines. An optional slash-delimited density (in  $\text{g}/\text{cm}^3$ ) may follow a species name. If no density is supplied, the unphysical value of  $-1.0$  is stored as a flag. The rules for bulk species symbols (names) are essentially the same as those for site species. [Figure 4.3: Examples of Bulk Data \(p. 65\)](#) shows sample bulk data. The rules for bulk data are summarized in [Table 4.2: Summary of the Rules for Bulk Data \(p. 64\)](#).

**Table 4.2: Summary of the Rules for Bulk Data**

Rule	Description
1	Bulk data must start with a line containing the word <code>BULK</code> , and may be followed by a slash-delimited name for the bulk phase (i.e., <code>BULK/ name /</code> ).
2	The <code>BULK</code> declaration and/or bulk name must be followed by one or more bulk species declarations. Declaring a bulk phase with no bulk species is an error.
3	Bulk and bulk species names are composed of up to sixteen upper- or lower-case character symbols. The names cannot begin with the <code>+</code> , <code>=</code> , <code>#</code> , or a number; an ionic species name may end with one or more <code>+</code> or <code>-</code> signs; an embedded plus sign must be enclosed in parentheses ( <code>+</code> ). Names cannot include a slash ( <code>/</code> ).
4	All species names should be unique; duplicate species names will be ignored and a warning issued. A species name may not duplicate a name of a gas-phase species, a surface species, or another bulk species.
5	All phase names must be unique. For example, a bulk phase name may not duplicate the name of any other phase (gas, surface site, or bulk phase).
6	Each bulk species that subsequently appears in a surface reaction must have been declared in this section.
7	A bulk species declaration may start anywhere on the line.
8	A bulk species name may be followed by an optional slash-delimited mass density (in $\text{g}/\text{cm}^3$ ).



Rule	Description
9	A bulk species declaration that begins on one line may not continue to the next line (i.e., do not break species names into two lines).
10	There may be more than one set of BULK data.
11	All characters on a line following an exclamation mark are considered comments and are ignored.
12	BULK data are not required.

**Figure 4.3: Examples of Bulk Data**

```

BULK / GA_RICH / GA2AS(1)/3.0/ GA3AS(1)/3.0/      END
                                           !an END statement is optional

BULK / GA_RICH /
GA2AS(1)/3.0/
GA3AS(1)/3.0/
GA2AS(1)/2.0/      !THIS NAME IS A DUPLICATE AND WILL BE IGNORED
BULK AS(B)          !BULK PHASE WITH NO NAME SUPPLIED
                   !ONLY ONE BULK SPECIES AND NO DENSITY SUPPLIED
END

```

## 4.4. Thermodynamic Data

Any chemical species that appears in a problem must have thermodynamic data associated with it. This data is used in evaluation of thermodynamic properties (entropy, enthalpy, heat capacity) and reverse reaction rate constants through the equilibrium constant. Often thermodynamic data for a species, for instance a surface species, is unknown. Such data can sometimes be calculated via theoretical techniques. However, the user can work around the need for actual thermodynamic data for all species by making the reactions irreversible. In this case, the user can supply “dummy” thermodynamic data for the surface species to satisfy the requirement.

### Note:

If every reaction in the mechanism is either irreversible, or if Arrhenius rate parameters are given explicitly for the reverse reaction, then the thermodynamic data for species are not actually used for anything related to the kinetics. They may, however, be used in surface heat balances if such are enabled for a particular reacting-flow problem.

The data may be extracted from a database file (e.g. *therm.dat*) and/or read directly from the *Surface Kinetics* input file. Details on the thermodynamic data format, whether including in the *Surface Kinetics* input file or in a thermodynamic database file, are provided in [Thermodynamic Data Format \(p. 3\)](#).

### Note:

When thermodynamic data is included in the *Surface Kinetics* Input file, it must immediately follow phase (SITE and BULK) data.

## 4.5. Reaction Mechanism Description

The surface reaction mechanism may consist of any number of chemical reactions involving the solid species named in the site and bulk data, as well as the gas-phase species declared in the *Gas-phase Kinetics* input file. A reaction may be reversible or irreversible. Reaction data must start with a line containing the word REACTIONS (or REAC). The lines following the REACTIONS line contain reaction descriptions together with their Arrhenius rate coefficients. The reaction description is composed of reaction data and perhaps optional auxiliary reaction data.

### 4.5.1. REACTIONS Line Options

On the same line as the REACTIONS word, you may define certain options that will apply globally to all surface reactions. In some cases, Auxiliary Reaction Keywords given for a specific reaction may override these global settings. A summary of the REACTIONS -line options are provided in [Table 4.3: Alphabetical Listing of REACTIONS-line Options for Surface Reaction Data \(p. 66\)](#).

---

#### Note:

Even if the default energy units are changed by giving one of these keywords, the temperature appearing in the Arrhenius expression of [Equation 3.5](#), i.e., in  $T$  raised to the  $\beta$  power and in the denominator of the activation energy term, is still in Kelvins.

---

#### Note:

If units are not specified,  $A_i$  and  $E_i$  are assumed to be in (cm, mole, sec, K) and cal/mole, respectively.

---

**Table 4.3: Alphabetical Listing of REACTIONS-line Options for Surface Reaction Data**

Keyword	Definition
ATM	Supersedes the default units for all surface reactions that follow the REACTIONS header line for pre-exponential factors $A_i$ ; the units of gas species are partial pressures in atm.
	<b>Notes</b>  Default units for $A_i$ are cgs (cm, sec, K, mole), the exact units depending on the order of the reaction.
BAR	Supersedes the default units for all surface reactions that follow the REACTIONS header line for pre-exponential factors $A_i$ ; the units of gas species are partial pressures in bar.
	<b>Notes</b>  Default units for $A_i$ are cgs (cm, sec, K, mole), the exact units depending on the order of the reaction.

Keyword	Definition
CAL/[MOLE]	<p>Re-iterates the default units for all surface reactions that follow the REACTIONS header line for parameters with energy units such as <math>E_i</math>.</p> <p><b>Notes</b></p> <p>Default units for <math>E_i</math> are cal/mole.</p>
DYN[ES]	<p>Supersedes the default units for all surface reactions which follow the REACTIONS header line for pre-exponential factors <math>A_i</math>; the units of gas species are partial pressures in dyne/cm<sup>2</sup>.</p> <p><b>Notes</b></p> <p>Default units for <math>A_i</math> are cgs (cm, sec, K, mole), the exact units depending on the order of the reaction.</p>
EVOL[TS]	<p>Supersedes the default units for all surface reactions which follow the REACTIONS header line for parameters with energy units such as <math>E_i</math>.</p> <p><b>Notes</b></p> <p>Default units for <math>E_i</math> are cal/mole.</p>
JOUL[ES/MOLE]	<p>Supersedes the default units for all surface reactions which follow the REACTIONS header line for parameters with energy units such as <math>E_i</math>.</p> <p><b>Notes</b></p> <p>Default units for <math>E_i</math> are cal/mole.</p>
KCAL/[MOLE]	<p>Supersedes the default units for all surface reactions which follow the REACTIONS header line for parameters with energy units such as <math>E_i</math>.</p> <p><b>Notes</b></p> <p>Default units for <math>E_i</math> are cal/mole.</p>
KELV[INS]KCAL / MOLE	<p>Supersedes the default units for all surface reactions which follow the REACTIONS header line for parameters with energy units such as <math>E_i</math>.</p> <p><b>Notes</b></p>

Keyword	Definition
	Default units for $E_i$ are cal/mole.
KJOU[LES/MOLE]	Supersedes the default units for all surface reactions which follow the REACTIONS header line for parameters with energy units such as $E_i$ .
	<b>Notes</b> Default units for $E_i$ are cal/mole.
MAXSP	Increases the maximum number of reactants or products allowed in a reaction. The number given by this keyword must be greater than the default limit of 6. For example, REACTIONS MAXSP=11.
	<b>Notes</b> This keyword is available to both the gas-phase and surface reaction mechanism.
MOLEC[ULES]	Supersedes the default units for all surface reactions which follow the REACTIONS header line for pre-exponential factors $A_i$ .
	<b>Notes</b> Default units for $A_i$ are cgs (cm, sec, K, mole), the exact units depending on the order of the reaction.
MOLE[S]	Re-iterates the default units for all surface reactions which follow the REACTIONS header line for pre-exponential factors $A_i$ .
	<b>Notes</b> Default units for $A_i$ are cgs (cm, sec, K, mole), the exact units depending on the order of the reaction.
MWOFF	Turns off the Motz-Wise correction of Equation 4.15 of the Chemkin-Pro Theory Manual for all sticking-coefficient reactions which follow the REACTIONS header line.
	<b>Notes</b> By default, the Motz-Wise correction is off for all sticking coefficient reactions; the default may be superseded for a particular sticking-coefficient reaction by use of the auxiliary reaction keyword MWOFF or MWON.
MWON	Turns on the Motz-Wise correction of Equation 4.15 of the Chemkin-Pro Theory Manual for all sticking-coefficient reactions which follow the REACTIONS header line.

Keyword	Definition
	<p><b>Notes</b></p> <p>By default, the Motz-Wise correction is off for all sticking coefficient reactions; the default may be superseded for a particular sticking-coefficient reaction by use of the auxiliary reaction keyword <b>MWOFF</b> or <b>MWON</b>.</p>
NONCON	Allows non-conservation of sites in any surface reaction which follows the REACTIONS header line. Normally, any reaction that does not conserve the number of surface sites in each surface phase is considered to be in error; the inclusion of NONCON on the REACTIONS line supersedes that rule.
PAS[CALS]	<p>Supersedes the default units for all surface reactions that follow the REACTIONS header line for pre-exponential factors <math>A_i</math>; the units of gas species are partial pressures in pascals.</p> <p><b>Notes</b></p> <p>Default units for <math>A_i</math> are cgs (cm, sec, K, mole), the exact units depending on the order of the reaction.</p>
SITE[FR]	<p>Supersedes the default units for all surface reactions which follow the REACTIONS header line for pre-exponential factors <math>A_i</math>; the units of surface species are site fraction and the reaction rate unit is 1/sec.</p> <p><b>Notes</b></p> <p>Default units for <math>A_i</math> are cgs (cm, sec, K, mole), the exact units depending on the order of the reaction.</p>
TOR[R]	<p>Supersedes the default units for all surface reactions which follow the REACTIONS header line for pre-exponential factors <math>A_i</math>; the units of gas species are partial pressures in torr.</p> <p><b>Notes</b></p> <p>Default units for <math>A_i</math> are cgs (cm, sec, K, mole), the exact units depending on the order of the reaction.</p>
USRPROD	The net rate-of-production for all species will be obtained by calling a user-supplied subroutine, SKUPROD. An optional slash(/)-delimited integer parameter allows the user to select from more than one type of rate formulation. Wherever the net rates of production of species are required, they will be obtained by calling the user-written subroutine. A template of SKUPROD is provided in the ANSYS Chemkin-Pro installation, in the file <i>sklib_user_routines.f</i> located in the

Keyword	Definition
	directory <i>user_subroutines</i> . Information about how to compile and link user routines into Chemkin-Pro is included in <a href="#">Chemkin-Pro Application Programming Interface Manual</a> .
	<b>Notes</b>  USRPROD cannot be used in conjunction with <a href="#">USRPROG</a> (entered after a particular reaction).

**Note:**

Chemkin-Pro does not support user-written programs, so you are cautioned to use the SKUPROD user routine feature at your own risk. Also, there are some features in the program executables that will be incompatible with the global replacement of species rates of production, such as sensitivity analysis and rate-of-production analysis. Such features will return zero values when user-rate programming is encountered.

## 4.5.2. Reaction Data

Each reaction entry is divided into two fields, (an entry may use multiple lines if it is more than 80 characters long). A reaction data entry is continued on the next line using the special character "& " at the end of the line; any information following the & symbol on the same line is ignored. The first field in the reaction entry contains the symbolic description of the reaction, while the second contains the Arrhenius rate coefficients. Both fields are format free, and blank spaces are ignored. All characters on a line following an exclamation mark (!) are considered comments and are ignored. Blank lines are also ignored.

The reaction description, given in the first field, must be composed of the species symbols, coefficients, and delimiters as summarized below.

**Table 4.4: Surface Reaction Data Criteria**

Species Symbols	
Each species in a reaction is described with the unique sequence of characters as they appear in the species data and the thermodynamic data.	
Coefficients	
A species symbol may be preceded by an integer or real coefficient. The coefficient has the meaning that there are that many moles of the particular species present as either reactants or products; e.g., 2OH is equivalent to OH +OH. The "# " symbol is used to mark stoichiometric coefficients that are additionally multiplied by a YIELD coefficient. This is explained in <a href="#">Auxiliary Reaction Data (p. 72)</a> .	
Delimiters	
+	A plus sign is the delimiter between each reactant species and each product species.
=	An equality sign is the delimiter between the last reactant and the first product in a reversible reaction.

Species Symbols	
<=>	An equality sign enclosed by angle brackets can also be used as the delimiter between the last reactant and the first product in a reversible reaction.
=>	An equality sign with an angle bracket on the right is the delimiter between the last reactant and the first product in an irreversible reaction.

The second field of the reaction line is used to define the Arrhenius rate coefficients  $A_i$ ,  $\beta_i$ , and  $E_i$  in that order, as given by [Equation 3.5 of the Chemkin-Pro Theory Manual](#). At least one blank space must separate the last species name in the reaction and first number. The three numbers must be separated by at least one blank space, be stated in either integer, floating point, or "E" format (e.g., 123 or 123.0 or 12.3E1), and have units associated with them (although the units do not appear on the input line). Unless modified by the REACTIONS line or by the UNITS auxiliary keyword, the default units for  $A_i$  are cgs (cm, sec, K, mole), the exact units depending on the order of the reaction. The factor  $\beta_i$  is dimensionless. The default units for the activation energies are cal/mole.

The second field of the reaction line may optionally be used to specify the coefficients  $a_i$ ,  $b_i$ , and  $c_i$  of [Equation 4.10 of the Chemkin-Pro Theory Manual](#) for a sticking coefficient. In order for the second field to apply to sticking coefficient parameters, the next line of input must contain the auxiliary keyword STICK.

Examples of some reaction data are shown in [Figure 4.4: Examples of Reaction Data \(p. 71\)](#). [Table 4.5: Summary of the Rules for Reaction Data \(p. 71\)](#) summarizes the reaction data rules.

**Figure 4.4: Examples of Reaction Data**

```
REACTIONS  KCAL/MOLE NONCON
ASH3 + AS(P) <=> ASH3(P) + AS(D)      4.0E11    0 25    ! Ref. 21
! ASH3 + AS(P) <=> ASH3(P) + AS(D)      4.0E11    0 0    ! same as previous
ASH <=> AS(D) + H(S)      1.0    0 0
      STICK
GA(CH3)3(L) + GA2AS(A) <=> AS + GA(CH3)(L) + 2 GAME & ! continued on next line
                                1.0E13    0 4000.
```

**Table 4.5: Summary of the Rules for Reaction Data**

Rule	Description
1	The first reaction line must start with the word REACTIONS (or REAC), and may be followed by units definition(s), the word MWON, MWOFF, NONCON, or the word USRPROD.
2	The word MWOFF can be used to turn off the Motz-Wise correction of <a href="#">Equation 4.15 of the Chemkin-Pro Theory Manual</a> , for all sticking-coefficient reactions, or the word MWON can be used to specify that the Motz-Wise correction is to be used for all sticking-coefficient reactions (the default). Including MWOFF or MWON as an auxiliary keyword for an individual reaction (discussed later) will override the setting given on the REACTIONS line.
3	Valid unit declarations are EVOLTS, KELVINS, CAL/MOLE, KCAL/MOLE, JOULES/MOLE, KJOULES/MOLE, MOLES, MOLECULES, SITEFR, ATM, BAR, DYN, TOR, and PASCAL.
4	The word NONCON is required on the first reaction line if any of the reactions do not conserve the number of surface sites of a given type.

Rule	Description
5	The reaction description can begin anywhere on this line. All blank spaces, except those separating the Arrhenius coefficients, are ignored.
6	Each reaction description must have =, <=>, or => between the last reactant and the first product.
7	Each species in a reaction is described with a unique sequence of characters (name) as they appear in the species data and the thermodynamic data. However, if a species name is not unique (because it is duplicated in another phase), the name must be modified by appending its slash-delimited phase name, i.e. as name / phase /.
8	Stoichiometric coefficients are represented by an integer or real number preceding a species name. The default is to assume a stoichiometric coefficient of 1. The "# " symbol preceding the stoichiometric coefficient denotes a coefficient which is additionally multiplied by a "yield" multiplier.
9	A reaction description may be contained on more than one line. If a line contains the symbol &, all information following the & symbol will be ignored and the next line will be considered a continuation of the first.
10	Three Arrhenius coefficients must appear in order ( $A_i$ , $\beta_i$ , and $E_i$ ) on each Reaction line, separated from each other and from the reaction description by at least one blank space; no blanks are allowed within a number.
11	There cannot be more than six reactants or six products in a reaction.
12	To specify a sticking coefficient rather than a rate constant the three numbers after the reaction description have the meaning $a_i$ , $b_i$ , and $c_i$ (see <a href="#">Equation 4.10 of the Chemkin-Pro Theory Manual</a> ) and the auxiliary reaction data word STICK must appear on the next line of input. To use this option the reaction must have only one gas-phase species as a reactant and its stoichiometric coefficient must be 1.
13	All characters on a line following an exclamation mark are comments.
14	For best results, an END statement should follow reaction input.

### 4.5.3. Auxiliary Reaction Data

Auxiliary information appears on one or more separate lines after the reaction data line is read, and serves to modify or give additional parameters needed to evaluate that reaction's rate expression. The format in an auxiliary information line is a character string keyword followed by a slash-delimited (/) field containing an appropriate number of parameters (either integer, floating point, E format, or character). Examples of many of the auxiliary options described in this section are shown in [Figure 4.5: Examples of Auxiliary Reaction Data \(p. 81\)](#) . [Table 4.6: Alphabetical Listing of Surface Reaction Auxiliary Keywords \(p. 72\)](#) provides detailed information on the meaning and usage of each auxiliary keyword entry that may be included as part of the Surface Reaction Data.

**Table 4.6: Alphabetical Listing of Surface Reaction Auxiliary Keywords**

Keyword	Definition
BOHM	<b>Bohm Velocity Limit for Ions</b> - Applies the Bohm velocity correction for a reaction involving a positive ionic species (see <a href="#">Equation 4.29 of the Chemkin-Pro Theory Manual</a> ). No auxiliary parameters are required.



Keyword	Definition			
	Reaction Example	CL+ + E                    => CL                    0.4            0.0 0.0  BOHM		
	Notes	<ul style="list-style-type: none"><li>• The three coefficients given in the second field of the reaction line are interpreted as the parameters <math>a_i, b_i, c_i</math> in Equation 4.29 of the Chemkin-Pro Theory Manual ).</li><li>• The reaction can have only one gas-phase reactant species, which must be a positive ion, and its stoichiometric coefficient must be 1.</li></ul>		
COV	<b>Coverage Dependent Reactions</b> - Modifies the expression for the forward rate constant by coverage parameters (see Equation 4.7 of the Chemkin-Pro Theory Manual ). Must be followed by (slash delimited) surface species name and the three parameters $\eta_{ki}, \mu_{ki}$ and $\varepsilon_{ki}$ .			
	Parameters	Optional/Reqd.	Units	Examples
	Species name	Required	--	COV /Pt(S) 0.0 0.0 0.9/
	Coverage parameter $\eta_{ki}$	Required	--	COV /Pt(S) <b>0.0</b> 0.0 0.9/
	Coverage parameter $\mu_{ki}$	Required	--	COV /Pt(S) 0.0 <b>0.0</b> 0.9/
	Coverage parameter $\varepsilon_{ki}$	Required	cal/mole	COV /Pt(S) 0.0 0.0 <b>0.9</b> /
	Reaction Example	O(S) +O(S) =>Pt(S) +Pt(S) +O2 3.700E+23 0.0 213.0  COV/O(S) 0.0 0.0 -93.3/		
	Notes	<ul style="list-style-type: none"><li>• More than one set of COV data can appear for a given reaction, and these would be applied multiplicatively as in Equation 4.7 of the Chemkin-Pro Theory Manual .</li></ul>		
DCOL	The reaction rate is proportional to the collision frequency between a gas molecule and a particle surface (see Equation 18.79 of the Chemkin-Pro Theory Manual ). Must be followed by the (slash delimited) collision-diameter of the gas-phase reactant.			
	Parameters	Optional/Reqd.	Units	Examples
	Collision diameter	Required	cm	DCOL / <b>2.45E-8</b> /
	Reaction Example	Al + 8H(se) => 5H(se) + 6C(B) + 3open(se) + 4H2 + H 0.1 0.0 0.0  FORD/H(se) 2.0/  DCOL/2.46E-8/  STICK		

Keyword	Definition			
	Notes	<ul style="list-style-type: none"><li>• The reaction must be irreversible.</li><li>• The reaction may have only one gas-phase.</li></ul>		
DUP	<b>Duplicate Reactions</b> - Two or more reactions can involve the same set of reactants and products, but proceed through distinctly different processes. In these cases, it may be appropriate to state a reaction mechanism that has two or more reactions that are the same, but have different rate parameters. However, duplicate reactions are normally considered errors by the <i>Surface Kinetics</i> Pre-Processor. If the user requires duplication (e.g., the same reactants and products with different Arrhenius parameters), keyword DUP must follow the reaction line of each duplicate reaction (including the first occurrence of the reaction that is duplicated). For example, if the user wishes to specify different rate expressions for each of two identical reactions, there must be two occurrences of the DUP keyword, one following each of the reactions. No auxiliary parameters are required.			
	Reaction Example	<pre>O2 + 2PT(S) =&gt; 2O(S)           1.80E+21      -0.5      0.0  DUP  O2 + 2PT(S) =&gt; 2O(S)           0.023      0.00      0.00  DUP</pre>		
	Notes	DUP is required for each of any duplicated reaction in the mechanism.		
ENRGDEP	<b>Ion-energy Dependent Rates</b> - Allows the rate constant to depend on ion energy according to <a href="#">Equation 4.30</a> of the <a href="#">Chemkin-Pro Theory Manual</a> . ENRGDEP must be followed by the three (slash delimited) $E_{ion,0}$ , $f_i$ , and $g_i$ .			
	Parameters	Optional/Reqd.	Units	Examples
	Threshold energy $E_{ion,0}$	Required	cal/mole	ENRGDEP / <b>1.0</b> 0.5 1.0/
	Exponential constant $f_i$	Required	--	ENRGDEP /1.0 <b>0.5</b> 1.0/
	Exponential constant $g_i$	Required	--	ENRGDEP /1.0 0.5 <b>1.0</b> /
	Reaction Example	<pre>E + CL+ + SICL3(S) + SI(B) =&gt; SICL4 + SI(S)          0.50      0.0      0.  BOHM  ENRGDEP/1. 0.5 1.0/  UNITS/EVOLT/</pre>		
	Notes	<ul style="list-style-type: none"><li>• There must be exactly one positive ionic reactant species in the reaction.</li><li>• Only irreversible reactions are allowed with this option.</li></ul>		

Keyword	Definition			
FORD	<b>Arbitrary Reaction Orders</b> - Supersedes the forward reaction order for any species in the mechanism (with respect to species concentration), regardless of whether the species appears as a reactant or a product in the reaction. FORD is followed, in slash-delimited format, by the species name and the new reaction order. This option overrides the values of $\nu_{ki}$ in Equation 3.4 of the Chemkin-Pro Theory Manual pertaining to the particular species named on the line; the reaction order for all other species is maintained at the default values.			
	Parameters	Optional/Reqd.	Units	Examples
	Species name	Required	--	FORD /Pt(S) 1.0/
	Stoichiometric coefficient	Required	--	FORD /Pt(S) <b>1.0</b> /
	Reaction Example	A1 + 8H(se) => 5H(se) + 6C(B) + 3open(se) + 4H2 + H    0.1    0.0    0.0  FORD/H(se) 2.0/  DCOL/2.46E-8/  STICK		
	Notes	• Multiple occurrences of the FORD construct may appear on the auxiliary line.		
LANG	<b>Langmuir-Hinshelwood Reaction Parameters</b> - Indicates the use of the Langmuir-Hinshelwood rate expression. One auxiliary line should be supplied for each species appearing in the denominator of Equation 4.21 of the Chemkin-Pro Theory Manual . The keyword is followed, in slash delimited format, by the species name, the pre-exponential multiplier, the temperature factor, the enthalpy for the equilibrium constant, and the reaction order for that species (usually equal to one). The equilibrium constant is defined as $K=AT^{\beta}\exp(-H/RT)$ , similar to the standard expression for rate constants.			
	Parameters	Optional/Reqd.	Units	Examples
	Species name	Required	--	LANG /C6H6 1.26 0.0 0.0 1.0/
	Pre-exponential factor A	Required	Depends on reaction	LANG /C6H6 <b>1.26</b> 0.0 0.0 1.0/
	Temperature exponent $\beta$	Required	--	LANG /C6H6 1.26 <b>0.0</b> 0.0 1.0/
	Equilibrium enthalpy H	Required	cal/mole	LANG /C6H6 1.26 0.0 <b>0.0</b> 1.0/
	Reaction order	Required	--	LANG /C6H6 1.26 0.0 0.0 <b>1.0</b> /
	Reaction Example	C6H5CH3 + H2 => C6H6 + CH4  2.507E-8    0.0    0.0    ! rate at 600C		

Keyword	Definition			
		LANG /C6H6 1.26 0.0 0.0 1.0/  LANG /C6H5CH3 1.01 0.0 0.0 1.0/  LHDE /1/  LHNU /C6H5CH3/  LHPR /atm/		
	Notes	<ul style="list-style-type: none"><li>• Only irreversible reactions are allowed with this option.</li><li>• Each species listed in a LHNU statement must have a LANG statement.</li><li>• Additional keywords LHDE , LHNU , and LHPR provide more flexibility in the form of the Langmuir-Hinshelwood or Eley-Rideal rate expressions.</li></ul>		
LHDE	<b>Langmuir-Hinshelwood Denominator Exponent Parameter</b> - Allows the default value of 2 for the overall exponent for the denominator ( <i>m</i> ) to be overridden when LANG is used to specify a Langmuir-Hinshelwood rate expression. To specify an Eley-Rideal reaction, this keyword would be used and <i>m</i> set to 1. The use of any positive number is permitted, including real or fractional numbers.			
	Parameters	Optional/Reqd.	Units	Examples
	Denominator exponent <i>m</i>	Required	--	LHDE /1/
	Reaction Example	C6H5CH3 + H2 => C6H6 + CH4  2.507E-8 0.0 0.0 ! rate at 600C  LANG /C6H6 1.26 0.0 0.0 1.0/  LANG /C6H5CH3 1.01 0.0 0.0 1.0/  LHDE /1/  LHNU /C6H5CH3/  LHPR /atm/		
LHNU	Allows the explicit inclusion of equilibrium constants in the numerator of the LANG rate expression (the use of <i>k</i> rather than <i>k'</i> , see Langmuir-Hinshelwood and Eley-Rideal Reactions of the Chemkin-Pro Theory Manual ) when LANG is used to specify a Langmuir-Hinshelwood rate expression. This keyword is followed by a slash delimited list of species names. For each species in the list, a multiplier of <i>K</i> will be applied to the rate constant.			
	Parameters	Optional/Reqd.	Units	Examples
	Species name	Required	--	LHNU /C6H5CH3/
	Reaction Example	C6H5CH3 + H2 => C6H6 + CH4		

Keyword	Definition			
		<pre>2.507E-8    0.0    0.0    ! rate at 600C  LANG /C6H6    1.26    0.0    0.0    1.0/  LANG /C6H5CH3    1.01    0.0    0.0    1.0/  LHDE /1/  LHNU /C6H5CH3/  LHPR /atm/</pre>		
	Notes	<ul style="list-style-type: none"><li>Each species listed in a LHNU statement must have a LANG statement.</li></ul>		
LHPR	Indicates that the equilibrium constants are given in pressure units when LANG is used to specify a Langmuir-Hinshelwood rate expression. The LHPR keyword will affect the equilibrium constants for the specified reaction only; the reaction rate will still be assumed to be in the units specified on the REACTIONS line, or in the default moles, cm, and sec. The keyword is followed by the slash-delimited name of the pressure unit being used: ATM, BAR, TORR, PASC (for Pascals), or DYNE (for dynes per square cm), where the names are not case sensitive.			
	Parameters	Optional/Reqd.	Units	Examples
	Pressure units character string	Required	--	LHPR /atm/
	Reaction Example	<pre>C6H5CH3 + H2 =&gt; C6H6 + CH4  2.507E-8    0.0    0.0    ! rate at 600C  LANG /C6H6    1.26    0.0    0.0    1.0/  LANG /C6H5CH3    1.01    0.0    0.0    1.0/  LHDE /1/  LHNU /C6H5CH3/  LHPR /atm/</pre>		
MWOFF	Motz-Wise Correction - Turns off the Motz-Wise correction of Equation 4.15 of the Chemkin-Pro Theory Manual for a sticking-coefficient reaction.			
	Reaction Example	<pre>AR* =&gt; AR          1.0    0.0    0.0  STICK  MWOFF</pre>		
	Notes	<ul style="list-style-type: none"><li>By default, the Motz-Wise correction will be off for all sticking coefficient reactions; the default may be changed by including the keyword MWON on the REACTIONS line.</li></ul>		

Keyword	Definition			
MWON	<b>Motz-Wise Correction</b> - Turns on the Motz-Wise correction of <a href="#">Equation 4.15</a> of the <a href="#">Chemkin-Pro Theory Manual</a> for a sticking-coefficient reaction, superseding the default. By default the Motz-Wise will be off for all reactions using sticking coefficients unless the MWON keyword is given on the REACTIONS line, in which the new default will be to include the correction term.			
	<b>Reaction Example</b>	<pre>ALMe3 + O(S) =&gt; ALMe2(S) + 0.5C2H6 0.1      0.0      0.0  STICK  MWON</pre>		
	<b>Notes</b>	<ul style="list-style-type: none"><li>By default, the Motz-Wise correction will be off for all sticking coefficient reactions; the default may be changed by including the keyword MWON on the REACTIONS line.</li></ul>		
NATIVE	Indicates the native species of a particle; see <a href="#">Native Surface Sites</a> of the <a href="#">Chemkin-Pro Theory Manual</a> .			
	<b>Reaction Example</b>	<pre>OPEN(S) /NATIVE/</pre>		
NUCL	Supersedes the default rate calculation with the nucleation reaction rate expression; see <a href="#">Nucleation Reaction Data</a> of the <a href="#">Chemkin-Pro Theory Manual</a> .			
	<b>Reaction Example</b>	<pre>2A4 =&gt; 32C(B) + 20 H(se) + 28.72 open(se)          1.0E10    0.5    0.0  NUCL</pre>		
REV	<b>Reverse Reaction Parameters</b> - Supersedes the reverse rates that would normally be computed through the equilibrium constant, <a href="#">Equation 3.6</a> of the <a href="#">Chemkin-Pro Theory Manual</a> . REV must be followed by the three slash-delimited Arrhenius coefficients ( $A_i$ , $\beta_i$ , and $E_i$ ) to specify the reverse rate.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Pre-exponential factor <math>A_i</math></i>		Depends on reaction	REV /1.0E13 0.0 15000./
	<i>Temperature exponent <math>\beta_i</math></i>		--	REV /1.0E13 0.0 15000./
	<i>Activation energy <math>E_i</math></i>		cal/mole	REV /1.0E13 0.0 15000./
	<b>Reaction Example</b>	<pre>C(S,R) + CH3 &lt;=&gt; D + CH3(S) 4.0E12    0.0    1200.0  REV /1.0E13 0.0 15000./</pre>		
RORD	<b>Arbitrary Reaction Orders</b> - Supersedes the reverse reaction order for any species in the mechanism (with respect to species concentration), regardless of whether the species appears as a reactant or a product in the reaction. RORD must be followed by the slash-delimited species name and the new reaction order, and supersedes the values of $\nu''_{ki}$ in <a href="#">Equation 3.4</a> of the <a href="#">Chemkin-Pro Theory Manual</a> pertaining to the particular species named on the line; the reaction order for all			

Keyword	Definition			
	other species maintain their default values. Multiple occurrences of the RORD construct may appear on the auxiliary line.			
	Parameters	Optional/Reqd.	Units	Examples
	Species name	Required	--	RORD /OH 2.0/
	Stoichiometric coefficient $\nu''_{ki}$	Required	--	RORD /OH 2.0/
	Reaction Example	H2+O2=2OH 0.170E+14 0.00 47780  RORD /OH 2.0/		
	Notes	• See also FORD .		
STICK	<b>Sticking Coefficients</b> - The three coefficients given in the second field of the reaction line are to be interpreted as the parameters $a_i$ , $b_i$ , and $c_i$ in Equation 4.10 of the Chemkin-Pro Theory Manual for a sticking coefficient (rather than as a rate constant). There can be only one gas-phase reactant species in a sticking-coefficient reaction; moreover, its stoichiometric coefficient must be 1.			
	Reaction Example	A1 + 8H(se) => 5H(se) + 6C(B) + 3open(se) + 4H2 + H 0.1 0.0 0.0  FORD/H(se) 2.0/  DCOL/2.46E-8/  STICK		
UNITS	<b>Unit Specifications for Reactions</b> - Supersedes the current units for a particular reaction rate fit that may differ from the default units specified for other reaction expressions in the chemistry mechanism. UNITS must be followed by the slash-delimited character-string <b>string</b> , where <b>string</b> is one of the following (letters in brackets are optional): Parameters with energy units such as $E_i$ : EVOL[TS], KELV[INS], CAL/[MOLE], KCAL/[MOLE], JOUL[ES/ MOLE], or KJOU[LES/MOLE]. Pre-exponential factors $A_i$ : MOLE[S] or MOLEC[ULES], where the inclusion of MOLEC would indicate that the reaction rate expression is in units of molecules/cm <sup>3</sup> rather than mole/cm <sup>3</sup> . ATM, BAR, PAS[CALS], DYN[ES], TOR[R] for pre-exponential factors $A_i$ , where the units of gas species are partial pressures. SITE[FR], where the units of surface species are site fractions and the rate units are 1/sec.			
	Parameters	Optional/Reqd.	Units	Examples
	Reaction units character string	Required	--	UNITS /MOLECUES/
	Reaction Example	CF3+ + E + #WSIO2(B) => #SIO2 + CF3 0.33 0.0 0.0  BOHM !  YIELD /0.01 20. 0.5 1.0/ UNITS/EVOLTS/		

Keyword	Definition		
	<b>Notes</b>	<ul style="list-style-type: none"><li>• Default units for <math>A_i</math> are cgs (cm, sec, K, mole), the exact units depending on the order of the reaction.</li><li>• Default units for <math>E_i</math> are cal/mole.</li><li>• Even if the default energy units are changed by giving the UNITS keyword, the temperature appearing in the Arrhenius expression of Equation 3.5 of the Chemkin-Pro Theory Manual , i.e., in T raised to the <math>\beta</math> power and in the denominator of the activation energy term, is still in Kelvins.</li><li>• If any of the units strings are given on the REACTIONS header line, it applies to all reactions, but may be superseded for a particular reaction by the auxiliary UNITS keyword.</li><li>• UNITS allows only one string parameter, but the user can repeat UNITS as many times as needed for a given reaction.</li></ul>	
USRPROG	<b>Optional User Rate Subroutine SKUPROG</b> – The net rate-of-progress for the reaction will be obtained by calling a user-supplied subroutine, SKUPROG. An optional slash(/)-delimited integer parameter allows the user to select from more than one type of rate formulation. Wherever the net reaction rate is required, it will be obtained by calling the user-written subroutine. A template of SKUPROG is provided in the ANSYS Chemkin-Pro installation, in the file <b>sklib_user_routines.f</b> located in the directory <b>user_subroutines</b> . Information about how to compile and link user routines into Chemkin-Pro is included in <a href="#">Chemkin-Pro Application Programming Interface Manual</a> .		
	Parameters	Optional/Reqd.	Units
	Rate formulation type	Optional	--
	Reaction Example	CH3OH +H2O => CO2 + 3H2                    1.0 0.00 0.0  USRPROG / 3 /	
	Notes	<ul style="list-style-type: none"><li>• USRPROG applies only to irreversible reactions, and cannot be used in conjunction with <a href="#">USRPROD</a> (entered on the REACTIONS header line).</li></ul>	
YIELD	<b>Ion-energy-dependent Yield</b> - Ion-enhanced reaction yield can be applied to a reaction using the following two steps. First, place a pound sign (#) in front of the species symbol (or stoichiometric coefficient if given) for each species that is subject to the ion-energy yield enhancement. The “sub-reaction” of species and coefficients demarcated with the # sign must satisfy mass, elemental, charge and site balance. Second, the auxiliary keyword YIELD must appear after the reaction, followed by the four parameters, $h_{\text{yield}}$ , $E_{\text{yield},0}$ , $t_{\text{ir}}$ , and $u_i$ (as described in Equation 4.33 of the <a href="#">Chemkin-Pro Theory Manual</a> ). These parameters are		



Keyword	Definition			
	included as a slash-delimited set following the YIELD auxiliary keyword. An example of a YIELD reaction is shown in <a href="#">Figure 4.5: Examples of Auxiliary Reaction Data (p. 81)</a> .			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Multiplicative factor</i> $h_{\text{yield}}$	Required	Depends on reaction	YIELD / <b>0.053</b> 4.0 0.5 1.0/
	<i>Energy threshold E</i> yield,0	Required	cal/mole	YIELD /0.053 <b>4.0</b> 0.5 1.0/
	<i>Exponential constant <math>t_i</math></i>	Required	--	YIELD /0.053 4.0 <b>0.5</b> 1.0/
	<i>Exponential constant <math>u_i</math></i>	Required	--	YIELD /0.053 4.0 0.5 <b>1.0</b> /
	<b>Reaction Example</b>	$\text{CF}_3^+ + \text{E} + \text{\#WSIO}_2(\text{B}) \Rightarrow \text{\#SIO}_2 + \text{CF}_3$ <p style="text-align: center;">0.33      0.0      0.0</p> <p>BOHM !</p> <p>YIELD /0.01 20. 0.5 1.0/ UNITS/EVOLTS/</p>		
	<b>Notes</b>	<ul style="list-style-type: none"> <li>A reaction declared with ion-enhanced yield must contain one (and only one) positive ionic reactant species.</li> </ul>		

**Note:**

Even if the default energy units are changed by giving one of the UNITS keyword, the temperature appearing in the Arrhenius expression of [Equation 3.5](#) of the [Chemkin-Pro Theory Manual](#) , i.e., in  $T$  raised to the  $\beta$  power and in the denominator of the activation energy term, is still in Kelvins.

### 4.5.3.1. Summary of Auxiliary Reaction Data

Any number of auxiliary information lines may follow a reaction line, in any order, and any number of keywords may appear on an auxiliary information line; however, an auxiliary keyword and its parameter(s) must appear on the same line.

Examples of auxiliary information are shown in [Figure 4.5: Examples of Auxiliary Reaction Data \(p. 81\)](#) . The above rules are summarized in [Table 4.7: Summary of the Rules for Auxiliary Reaction Data \(p. 82\)](#) .

**Figure 4.5: Examples of Auxiliary Reaction Data**

```

REACTIONS      KCAL/MOLE
! THE FOLLOWING ARE *CONTRIVED* EXAMPLES OF AUXILIARY KEYWORD USAGE
  SICL(S)  <=>  CL + SI(S)                                1.0E-3  0.0    2.
                                                    REV/1.0E13  0.0    37./
  CL + SICL(S) <=>  CL2 + SI(S)                            0.1     1.1    20.
    DUPLICATE      STICK
  RORD /SI(S)  0/

```

```

CL + SICL(S) <=> CL2 + SI(S) 1.4E11 0.0 15.
    DUPLICATE COV/SICL(S) -1.2 0.5 32./ FORD/CL+ 1.0/
CL* => CL 1.0 0.0 0.
    STICK MWOFF
E + CL+ + SICL3(S) + SI(B) => SICL4 + SI(S) 0.50 0.0 0.
    BOHM
    ENRGDEP/1. 0.5 1.0/ UNITS/EVOLT/
AR+ + E + #SIO2(D) => #SIO2 + AR 1.0 0.0 0.0
    BOHM
    YIELD /0.023052 35. 0.5 1.0/ UNITS/EVOLTS/
E + CL2+ + SICL3(S) + SI(B) => SICL4 + SICL(S) 0.50 0.0 0.0 FORD/ CL2+ 2.43/
C6H5CH3 + H2 => C6H6 + CH4 1.4E-8 0.0 0.0 ! rate at 600C
    LANG /C6H6 1.26 0.0 0.0 1.0/
    LANG /C6H5CH3 1.01 0.0 0.0 1.0/
    LHDE /1/
    LHNU /C6H5CH3/
    LHPR /atm/

```

**Table 4.7: Summary of the Rules for Auxiliary Reaction Data**

Rule	Description
1	Auxiliary information lines may follow a reversible reaction to specify the reverse rate parameters explicitly; auxiliary information must follow any reactions that are duplicated.
2	Auxiliary keyword declarations may appear anywhere on the line, in any order.
3	Any number of auxiliary keywords may appear on a line, and more than one line may be used, but a keyword and its parameter(s) must appear on the same line.
4	Multiple keywords appearing on the same line must be separated by at least one blank space.
5	Any blank spaces between a keyword and the first slash are ignored and any blanks between the slashes and parameter(s) are also ignored. However, no blank spaces are allowed within a keyword or parameter.
6	The keyword REV followed by three slash-delimited Arrhenius coefficients may be used to specify the reverse rate parameters.
7	The keyword DUPLICATE (or DUP) must follow every occurrence of a duplicated reaction.
8	The keyword STICK indicates that the three coefficients on the reaction line are to be interpreted as the parameters $a_i$ , $b_i$ , and $c_i$ in Equation 4.10 of the <a href="#">Chemkin-Pro Theory Manual</a> . There must be exactly one gas-phase reactant species; its stoichiometric coefficient must be 1.
9	The keyword COV is used to modify the forward rate constant by the expression in Equation 4.7 of the <a href="#">Chemkin-Pro Theory Manual</a> . The word COV is followed by a surface species name and the three coverage parameters $\eta_{ki'}$ , $\mu_{ki}$ and $\varepsilon_{ki}$ . The four entries after the word COV are slash-delimited.
10	The keyword BOHM indicates that the three coefficients on the reaction line are to be interpreted as the parameters $a_i$ , $b_i$ , and $c_i$ in Equation 4.29 of the <a href="#">Chemkin-Pro Theory Manual</a> ; the Bohm velocity correction is applied. There must be exactly one gas-phase reactant species and that species must be a positive ionic species; its stoichiometric coefficients must be 1. Only irreversible reactions are allowed with this option. The electron must be declared in the list of species names in the <i>Gas-phase Kinetics</i> Pre-processor input.

Rule	Description
11	The keyword <code>ENRGDEP</code> allows the rate constant to depend on ion energy according to Equation 4.30 of the <a href="#">Chemkin-Pro Theory Manual</a> . The keyword is followed by the three parameters $E_{ion,0}$ , $f_i$ , and $g_i$ which are slash-delimited. There must be exactly one positive ionic reactant species in the reaction. Only irreversible reactions are allowed with this option.
12	The keywords <code>FORD</code> and <code>RORD</code> can be used to change the reaction order (with respect to species concentration) of the forward or reverse reaction, respectively, for any species in the mechanism, regardless of whether the species appears as a reactant or a product in the reaction. The species name and the new reaction order (slash-delimited) follow the keyword.
13	The <code>YIELD</code> keyword allows modification of the stoichiometric coefficients in a sub-reaction using the ion-yield option. The usage requires preceding each species in the sub-reaction (or its stoichiometric coefficient) with the pound sign (#). Following the reaction line, declare the <code>YIELD</code> keyword, then the four parameters $h_{yield}$ , $E_{yield,0}$ , $t_i$ , and $u_i$ of Equation 4.33 of the <a href="#">Chemkin-Pro Theory Manual</a> , between slashes. There must be exactly one positive ionic reactant species in the reaction. Only irreversible reactions are allowed with this option. The sub-reaction demarcated with the # symbols must satisfy mass, elemental, charge and site balance. An example of the <code>YIELD</code> keyword appears in <a href="#">Figure 4.5: Examples of Auxiliary Reaction Data (p. 81)</a> .
14	The <code>UNITS</code> keyword can be used to override the current default units for parameters with energy units or the pre-exponential factor for a given reaction. The usage is <code>UNITS/ <b>string</b> /</code> , where <b>string</b> is one of the following: <code>EVOLTS</code> , <code>KELVINS</code> , <code>CAL/MOLE</code> , <code>KCAL/MOLE</code> , <code>JOULES/MOLE</code> , or <code>KJOULES/MOLE</code> (for parameters with energy units), or <code>MOLES</code> or <code>MOLECULES</code> (for pre-exponential factors).
15	The string <code>MWON</code> can be used to turn on the Motz-Wise correction of Equation 4.15 of the <a href="#">Chemkin-Pro Theory Manual</a> or the string <code>MWOFF</code> can be used to turn off this correction for a sticking coefficient reaction. Using the <code>MWOFF</code> or <code>MWON</code> keyword overrides the default option set up on the <code>REACTIONS</code> line or the default supplied by <i>Surface Kinetics</i> (which is <code>MWOFF</code> ).
16	The <code>LANG</code> keyword can be used to input a Langmuir-Hinshelwood rate expression. The keyword is followed by a species name, three parameters giving the equilibrium constant, and a fourth parameter giving the order of that species in the reaction. Additional keywords <code>LHDE</code> , <code>LHNU</code> , and <code>LHPR</code> provide more flexibility in the form of the Langmuir-Hinshelwood or Eley-Rideal rate expressions.
17	The keyword <code>LHDE</code> allows the default value of 2 for the overall exponent for the denominator ( $m$ ) to be overridden when <code>LANG</code> is used to specify a Langmuir-Hinshelwood rate expression. To specify an Eley-Rideal reaction, this keyword would be used to set $m$ to 1. The use of any positive number is permitted, including real or fractional numbers.
18	The keyword <code>LHNU</code> allows the explicit inclusion of equilibrium constants in the numerator of the <code>LH</code> rate expression (the use of $k$ rather than $k'$ , see <a href="#">Langmuir-Hinshelwood and Eley-Rideal Reactions</a> of the <a href="#">Chemkin-Pro Theory Manual</a> ) when <code>LANG</code> is used to specify a Langmuir-Hinshelwood rate expression. This keyword is followed by a slash delimited list of species names. For each species in the list, a multiplier of $K$ will be applied to the rate

Rule	Description
	constant. Each species listed in a LHNU statement must have a LANG statement.
19	The keyword LHPR indicates that the equilibrium constants are given in pressure units when LANG is used to specify a Langmuir-Hinshelwood rate expression. The LHPR keyword will affect the equilibrium constants for the specified reaction only; the reaction rate will still be assumed to be in the units specified on the REACTIONS line, or in the default moles, cm, and sec. The keyword is followed by the name of the pressure unit being used: atm, bar, torr, Pasc (for Pascals), or dyne (for dynes per square cm), where the names are not case sensitive.

#### 4.5.4. Problems Having No Reactions

In some problems only information about the surface and bulk species is needed (e.g., chemical equilibrium computations). For these cases it is not necessary to include reaction data. The Pre-processor will create the linking file *surf.asc*, but it will not contain any reaction information. Therefore, no subroutines in the *Surface Kinetics* Subroutine Library that deal with chemical reactions (e.g., chemical production rates) will be used (although doing so would not generate an error; the production rates of all species would be returned as zero).

#### 4.5.5. Error Checks

Each input line is checked for proper syntax and diagnostic messages are written to the pre-processor output file if errors are encountered. If an error occurs, the pre-processor continues to read and diagnose the input, but an error flag is written to the Linking file and *Surface Kinetics* subroutine SKINIT will not initialize the work arrays. Therefore, the input must be error free before a Reactor Model can be run or before any of the *Surface Kinetics* subroutines can be called in a Reactor Model.

Possibilities for an error condition are as follows:

**Table 4.8: Error Checks**

Data Type	Possible Errors
Site and Bulk Species Data	A duplicated species symbol (name) is not considered a fatal error, but is eliminated from consideration and a warning diagnostic message is printed.
	No site density is found for a declared site, or the site density is negative.
	No thermodynamic data are found for a declared species.
	A site or bulk phase name duplicates another phase name (gas surface site, or bulk phase name).
	A phase or species name contains an illegal character.
	Site occupancy number is negative.
	Bulk density for a bulk species is negative.
Thermodynamic Data	Thermodynamic data are format sensitive and therefore provide possibilities for error if not formatted exactly as

Data Type	Possible Errors
	described by <a href="#">Table 2.1: Summary of the Rules for Thermodynamic Data (p. 4)</a> .
	An element in the thermodynamic data for a declared species is not included in the <i>Gas-phase Kinetics</i> Pre-processor input element data.
	With the THERMO ALL option, line 2 (of <a href="#">Table 2.1: Summary of the Rules for Thermodynamic Data (p. 4)</a> ) is not found.
Reaction Data	A delimiter =>, <=>, or = between the reactants and the products is not found.
	Three Arrhenius parameters are not found.
	Reactants and/or products species names are not properly delineated by a plus sign (+).
	A species listed as a reactant or product is not declared in the species data.
	A reaction does not satisfy elemental balance.
	The number of sites in a reaction does not balance and the word NONCON was not included on the first REACTIONS line.
	The charge of the reaction does not balance.
	A reaction is a duplicate not declared by the auxiliary data keyword DUP.
	There are more than six reactants or six products in a reaction.
Auxiliary Reaction Data	An unknown or misspelled keyword occurs.
	Parameters for a keyword are not enclosed in slashes.
	There are the wrong number of parameters for a keyword.
	REV is declared for an irreversible reaction.
	Pre-exponential factor for a sticking coefficient is negative.
	For a sticking-coefficient reaction, there is more than one gas-phase species, or the stoichiometric coefficient for the gas-phase species is not 1.
	More than one BOHM declaration appeared for a given reaction.
	BOHM keyword is given for a reversible reaction.
	A positive ionic species did not appear as a reactant or its stoichiometric coefficient was not 1 in a Bohm reaction.
	More than 1 positive ionic species was a reactant in a Bohm reaction.
	The electron species was not declared in the list of species in the <i>Gas-phase Kinetics</i> Pre-processor input.
	Invalid string given with the UNITS auxiliary keyword.
	More than one ENRGDEP declaration appeared for a given reaction.
	A positive ionic species did not appear as a reactant or its stoichiometric coefficient was not 1 in a ENRGDEP reaction.

Data Type	Possible Errors
	Wrong number of ENRGDEP parameters given.
	Invalid species name given for FORD or RORD auxiliary keywords.
	A reaction order value was not found with the FORD or RORD keyword.
	RORD given for an irreversible reaction.
	No species coefficients were demarcated with a # symbol for a YIELD reaction.
	YIELD keyword given for a reversible reaction.
	A positive ionic species did not appear as a reactant or its stoichiometric coefficient was not 1 in a YIELD reaction.
	Wrong number of YIELD parameters given.
	More than 1 positive ionic species was a reactant in a YIELD reaction.
	LANG is declared for a reversible reaction, or for the same reaction as STICK, COV, BOHM, YIELD, or ENRGDEP.
	USRPROG given for a USRPROD mechanism.
	USRPROG given for a reversible reaction.

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## Chapter 5: Transport Database

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In this section we list the database file that is currently included with the *Transport* software. While this database file is more of a historical record, we expect that users will want to add their own collection of data to suit their own needs.

The database file included with ANSYS Chemkin-Pro should not be viewed as the last word in transport properties. Instead, it is a good starting point from which a user will provide the best available data for his particular application. Some of the numbers in the database have been determined by computing “best fits” to experimental measurements of a macroscopic transport property (for example, viscosity). In other cases the Lennard-Jones parameters have been estimated following the methods outlined in Svehla.[7] (p. 345) In still other cases they have been determined by computational chemistry techniques.

### 5.1. Transport Data Format

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The first 16 columns in each line of the database are reserved for the species name. Presently ANSYS Chemkin-Pro is programmed to allow no larger than 16-character names. Columns 17 through 80 are free-format, and they contain the molecular parameters for each species. They are, in order:

1. An index indicating whether the molecule has a monatomic, linear or nonlinear geometrical configuration. If the index is 0, the molecule is a single atom. If the index is 1 the molecule is linear, and if it is 2, the molecule is nonlinear.
2. The Lennard-Jones potential well depth  $\varepsilon/k_B$  in Kelvins.
3. The Lennard-Jones collision diameter  $\sigma$  in angstroms.
4. The dipole moment  $\mu$  in Debye.
5. The polarizability  $\alpha$  in cubic angstroms.
6. The rotational relaxation collision number  $Z_{\text{rot}}$  at 298 K.
7. A “comment” line is one that has either a period ( . ), slash ( / ), or exclamation mark ( ! ) as the first non-blank character. In addition, on any line, any input that follows an exclamation mark is taken as a comment.

---

#### Note:

A Debye is  $10^{-18} \text{ cm}^3/2 \text{ ergs}^{1/2}$ .

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### 5.2. Including Transport Data in the Gas-phase Kinetics Input File

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ANSYS Chemkin-Pro allows you to optionally include transport data within the *Gas-phase Kinetics* Input File. This is similar to the options available for thermodynamic data. This option can be used to supplement or replace transport data that may be provided in a separate file (e.g., *tran.dat*). In addition, this

option may be particularly useful when reaction-rate constants are given in terms of the collision frequency (see the description of the COLLEFF keyword in [Table 3.7: Alphabetical Listing of Gas-phase Reaction Auxiliary Keywords \(p. 43\)](#) ). In such cases, the Lennard-Jones diameter, which is obtained from the transport data, is required for calculation of the collision frequency that is used to derive the reaction rate for those reactions. These are cases when transport data might not otherwise be required but the necessary data for specific species needed in the collision-frequency reactions may be included in the *Gas-phase Kinetics* Input File.

A full description of the syntax of this option is included in [Transport Data \(p. 38\)](#) .

## 5.3. Transport Data Included with CHEMKIN

[Table 5.1: Species in Transport Database \(p. 88\)](#) lists the species contained in the ANSYS Chemkin-Pro tran.dat file, which is included in every installation, as the corresponding data for each species.

**Table 5.1: Species in Transport Database**

Species Name	Geometry	$\epsilon/k_B$	$\sigma$	$\mu$	$\alpha$	$Z_{\text{rot}}$
Al2Me6	2	471.	6.71	0.0	0.0	1.0
AlMe3	2	471.	5.30	0.0	0.0	1.0
AR	0	136.500	3.330	0.000	0.000	0.000
AR*	0	136.500	3.330	0.000	0.000	0.000
AS	0	1045.5	4.580	0.000	0.000	0.000
AS2	1	1045.5	5.510	0.000	0.000	1.000
ASH	1	199.3	4.215	0.000	0.000	1.000
ASH2	2	229.6	4.180	0.000	0.000	1.000
ASH3	2	259.8	4.145	0.000	0.000	1.000
AsH3	2	259.8	4.145	0.000	0.000	1.000
BCL3	2	337.7	5.127	0.000	0.000	1.000
C	0	71.400	3.298	0.000	0.000	0.000
C-Si3H6	2	331.2	5.562	0.000	0.000	1.000
C2	1	97.530	3.621	0.000	1.760	4.000
C2F4	2	202.6	5.164	0.000	0.000	1.000
C2F6	2	194.5	5.512	0.000	0.000	1.000
C2H	1	209.000	4.100	0.000	0.000	2.500
C2H2	1	209.000	4.100	0.000	0.000	2.500
C2H2OH	2	224.700	4.162	0.000	0.000	1.000
C2H3	2	209.000	4.100	0.000	0.000	1.000
C2H4	2	280.800	3.971	0.000	0.000	1.500
C2H5	2	252.300	4.302	0.000	0.000	1.500
C2H5OH	2	362.6	4.53	0.000	0.000	1.000
C2H6	2	252.300	4.302	0.000	0.000	1.500
C2N	1	232.400	3.828	0.000	0.000	1.000



Species Name	Geometry	$\varepsilon/k_B$	$\sigma$	$\mu$	$\alpha$	$Z_{\text{rot}}$
C2N2	1	349.000	4.361	0.000	0.000	1.000
C2O	1	232.400	3.828	0.000	0.000	1.000
C3H2	2	209.000	4.100	0.000	0.000	1.000
C3H3	1	252.000	4.760	0.000	0.000	1.000
C3H4	1	252.000	4.760	0.000	0.000	1.000
C3H4P	1	252.000	4.760	0.000	0.000	1.000
C3H6	2	266.800	4.982	0.000	0.000	1.000
C3H7	2	266.800	4.982	0.000	0.000	1.000
C3H8	2	266.800	4.982	0.000	0.000	1.000
C4H	1	357.000	5.180	0.000	0.000	1.000
C4H2	1	357.000	5.180	0.000	0.000	1.000
C4H2OH	2	224.700	4.162	0.000	0.000	1.000
C4H3	1	357.000	5.180	0.000	0.000	1.000
C4H4	1	357.000	5.180	0.000	0.000	1.000
C4H6	2	357.000	5.180	0.000	0.000	1.000
C4H8	2	357.000	5.176	0.000	0.000	1.000
C4H9	2	357.000	5.176	0.000	0.000	1.000
C4H9	2	357.000	5.176	0.000	0.000	1.000
C5H2	1	357.000	5.180	0.000	0.000	1.000
C5H3	1	357.000	5.180	0.000	0.000	1.000
C5H5OH	2	450.000	5.500	0.000	0.000	1.000
C6H2	1	357.000	5.180	0.000	0.000	1.000
C6H5	2	412.300	5.349	0.000	0.000	1.000
C6H5(L)	2	412.300	5.349	0.000	0.000	1.000
C6H5O	2	450.000	5.500	0.000	0.000	1.000
C6H6	2	412.300	5.349	0.000	0.000	1.000
C6H7	2	412.300	5.349	0.000	0.000	1.000
CF	1	94.2	3.635	0.000	0.000	1.000
CF2	2	108.0	3.977	0.000	0.000	1.000
CF3	2	121.0	4.320	0.000	0.000	1.000
CF4	2	134.0	4.662	0.000	0.000	1.000
CH	1	80.000	2.750	0.000	0.000	0.000
CH2	1	144.000	3.800	0.000	0.000	0.000
CH2(S)	1	144.000	3.800	0.000	0.000	0.000
CH2(SING)	1	144.000	3.800	0.000	0.000	0.000
CH2CHCCH	2	357.000	5.180	0.000	0.000	1.000
CH2CHCCH2	2	357.000	5.180	0.000	0.000	1.000
CH2CHCH2	2	260.000	4.850	0.000	0.000	1.000

Species Name	Geometry	$\varepsilon/k_B$	$\sigma$	$\mu$	$\alpha$	$Z_{\text{rot}}$
CH2CHCHCH	2	357.000	5.180	0.000	0.000	1.000
CH2CHCHCH2	2	357.000	5.180	0.000	0.000	1.000
CH2CO	2	436.000	3.970	0.000	0.000	2.000
CH2F2	2	318.0	4.080	0.000	0.000	1.000
CH2HCO	2	436.000	3.970	0.000	0.000	2.000
CH2O	2	498.000	3.590	0.000	0.000	2.000
CH2OH	2	417.000	3.690	1.700	0.000	2.000
CH3	1	144.000	3.800	0.000	0.000	0.000
CH3CC	2	252.000	4.760	0.000	0.000	1.000
CH3CCCH2	2	357.000	5.180	0.000	0.000	1.000
CH3CCCH3	2	357.000	5.180	0.000	0.000	1.000
CH3CCH2	2	260.000	4.850	0.000	0.000	1.000
CH3CH2CCH	2	357.000	5.180	0.000	0.000	1.000
CH3CHCH	2	260.000	4.850	0.000	0.000	1.000
CH3CHO	2	436.000	3.970	0.000	0.000	2.000
CH3CO	2	436.000	3.970	0.000	0.000	2.000
CH3O	2	417.000	3.690	1.700	0.000	2.000
CH3OH	2	481.800	3.626	0.000	0.000	1.000
CH4	2	141.400	3.746	0.000	2.600	13.000
CH4O	2	417.000	3.690	1.700	0.000	2.000
CHF3	2	240.0	4.330	0.000	0.000	1.000
CL	0	130.8	3.613	0.000	0.000	1.000
CL-	0	130.8	3.613	0.000	0.000	1.000
CL2BNH2	2	337.7	5.127	0.000	0.000	1.000
CN	1	75.000	3.856	0.000	0.000	1.000
CN2	1	232.400	3.828	0.000	0.000	1.000
CNC	1	232.400	3.828	0.000	0.000	1.000
CNN	1	232.400	3.828	0.000	0.000	1.000
CO	1	98.100	3.650	0.000	1.950	1.800
CO2	1	244.000	3.763	0.000	2.650	2.100
DMG	2	675.8	5.22	0.000	0.000	1.000
E	0	850.	425.	0.000	0.000	1.000
F	0	80.000	2.750	0.000	0.000	0.000
F2	1	125.700	3.301	0.000	1.600	3.800
GA	0	2961.8	4.62	0.000	0.000	0.000
GACH3	2	972.7	4.92	0.000	0.000	1.000
GAH	1	335.5	4.24	0.000	0.000	1.000
GAME	2	972.7	4.92	0.000	0.000	1.000

Species Name	Geometry	$\varepsilon/k_B$	$\sigma$	$\mu$	$\alpha$	$Z_{\text{rot}}$
GAME2	2	675.8	5.22	0.000	0.000	1.000
GAME3	2	378.2	5.52	0.000	0.000	1.000
GaMe3	2	378.2	5.52	0.000	0.000	1.000
H	0	145.000	2.050	0.000	0.000	0.000
H2	1	38.000	2.920	0.000	0.790	280.000
H2ASCH3	2	408.0	4.73	0.000	0.000	1.000
H2C4O	2	357.000	5.180	0.000	0.000	1.000
H2CCCCH	2	357.000	5.180	0.000	0.000	1.000
H2CCCCH2	2	357.000	5.180	0.000	0.000	1.000
H2CCCH	2	252.000	4.760	0.000	0.000	1.000
H2CN	1	569.000	3.630	0.000	0.000	1.000
H2NO	2	116.700	3.492	0.000	0.000	1.000
H2O	2	572.400	2.605	1.844	0.000	4.000
H2O2	2	107.400	3.458	0.000	0.000	3.800
H2S	2	301.000	3.600	0.000	0.000	1.000
H2SISIH2	2	312.6	4.601	0.000	0.000	1.000
H3SISIH	2	312.6	4.601	0.000	0.000	1.000
HC2N2	1	349.000	4.361	0.000	0.000	1.000
HCCHCCH	2	357.000	5.180	0.000	0.000	1.000
HCCO	2	150.000	2.500	0.000	0.000	1.000
HCCOH	2	436.000	3.970	0.000	0.000	2.000
HCL	1	344.7	3.339	0.000	0.000	1.000
HCN	1	569.000	3.630	0.000	0.000	1.000
HCNO	2	232.400	3.828	0.000	0.000	1.000
HCO	2	498.000	3.590	0.000	0.000	0.000
HCO+	1	498.000	3.590	0.000	0.000	0.000
HE	0	10.200	2.576	0.000	0.000	0.000
HF	1	330.000	3.148	1.920	2.460	1.000
HF0	1	352.000	2.490	1.730	0.000	5.000
HF1	1	352.000	2.490	1.730	0.000	5.000
HF2	1	352.000	2.490	1.730	0.000	5.000
HF3	1	352.000	2.490	1.730	0.000	5.000
HF4	1	352.000	2.490	1.730	0.000	5.000
HF5	1	352.000	2.490	1.730	0.000	5.000
HF6	1	352.000	2.490	1.730	0.000	5.000
HF7	1	352.000	2.490	1.730	0.000	5.000
HF8	1	352.000	2.490	1.730	0.000	5.000
HNCO	2	232.400	3.828	0.000	0.000	1.000

Species Name	Geometry	$\varepsilon/k_B$	$\sigma$	$\mu$	$\alpha$	$Z_{\text{rot}}$
HNNO	2	232.400	3.828	0.000	0.000	1.000
HNO	2	116.700	3.492	0.000	0.000	1.000
HNOH	2	116.700	3.492	0.000	0.000	1.000
HO2	2	107.400	3.458	0.000	0.000	1.000
HOCN	2	232.400	3.828	0.000	0.000	1.000
HSO2	2	252.000	4.290	0.000	0.000	1.000
I*C3H7	2	266.800	4.982	0.000	0.000	1.000
I*C4H9	2	357.000	5.176	0.000	0.000	1.000
K	0	850.	4.25	0.000	0.000	1.000
K+	0	850.	4.25	0.000	0.000	1.000
KCL	1	1989.	4.186	0.000	0.000	1.000
KH	1	93.3	3.542	0.000	0.000	1.000
KO	1	383.0	3.812	0.000	0.000	1.000
KO2	2	1213.	4.69	0.000	0.000	1.000
KOH	2	1213.	4.52	0.000	0.000	1.000
N	0	71.400	3.298	0.000	0.000	0.000
N*C3H7	2	266.800	4.982	0.000	0.000	1.000
N2	1	97.530	3.621	0.000	1.760	4.000
N2H2	2	71.400	3.798	0.000	0.000	1.000
N2H3	2	200.000	3.900	0.000	0.000	1.000
N2H4	2	205.000	4.230	0.000	4.260	1.500
N2O	1	232.400	3.828	0.000	0.000	1.000
NCN	1	232.400	3.828	0.000	0.000	1.000
NCNO	2	232.400	3.828	0.000	0.000	1.000
NCO	1	232.400	3.828	0.000	0.000	1.000
NH	1	80.000	2.650	0.000	0.000	4.000
NH2	2	80.000	2.650	0.000	2.260	4.000
NH3	2	481.000	2.920	1.470	0.000	10.000
NNH	2	71.400	3.798	0.000	0.000	1.000
NO	1	97.530	3.621	0.000	1.760	4.000
NO2	2	200.000	3.500	0.000	0.000	1.000
O	0	80.000	2.750	0.000	0.000	0.000
O(Si(OC2H5)3)2	2	522.7	5.25	0.000	0.000	1.000
O2	1	107.400	3.458	0.000	1.600	3.800
O3	2	180.000	4.100	0.000	0.000	2.000
OH	1	80.000	2.750	0.000	0.000	0.000
OSi(OC2H5)2	2	522.7	7.03	0.000	0.000	1.000
PH3	2	251.5	3.981	0.000	0.000	1.000

Species Name	Geometry	$\varepsilon/k_B$	$\sigma$	$\mu$	$\alpha$	$Z_{\text{rot}}$
S	0	847.000	3.839	0.000	0.000	0.000
S*C4H9	2	357.000	5.176	0.000	0.000	1.000
S2	1	847.000	3.900	0.000	0.000	1.000
SH	1	847.000	3.900	0.000	0.000	1.000
SI	0	3036.	2.910	0.000	0.000	0.000
Si(OC2H5)4	2	522.7	7.03	0.000	0.000	1.000
SI(OC2H5)4	2	522.7	7.03	0.000	0.000	1.000
Si(OH)(OC2H5)3	2	522.7	7.03	0.000	0.000	1.000
SI(OH)(OC2H5)3	2	522.7	7.03	0.000	0.000	1.000
SI(OH)2(OC2H5)2	2	522.7	6.35	0.000	0.000	1.000
Si(OH)2(OC2H5)2	2	522.7	6.35	0.000	0.000	1.000
SI(OH)3(OC2H5)	2	522.7	5.75	0.000	0.000	1.000
SI(OH)4	2	522.7	5.25	0.000	0.000	1.000
SI2	1	3036.	3.280	0.000	0.000	1.000
SI2H2	2	323.8	4.383	0.000	0.000	1.000
SI2H3	2	318.2	4.494	0.000	0.000	1.000
SI2H4	2	312.6	4.601	0.000	0.000	1.000
SI2H5	2	306.9	4.717	0.000	0.000	1.000
SI2H6	2	301.3	4.828	0.000	0.000	1.000
SI3	2	3036.	3.550	0.000	0.000	1.000
SI3H8	2	331.2	5.562	0.000	0.000	1.000
SIF	1	585.0	3.318	0.000	0.000	1.000
SIF3	2	309.6	4.359	0.000	0.000	1.000
SIF3NH2	2	231.0	4.975	0.000	0.000	1.000
SIF4	2	171.9	4.880	0.000	0.000	1.000
SIH	1	95.8	3.662	0.000	0.000	1.000
SIH2	2	133.1	3.803	0.000	0.000	1.000
SIH2(3)	2	133.1	3.803	0.000	0.000	1.000
SIH3	2	170.3	3.943	0.000	0.000	1.000
SIH3SIH2SIH	2	331.2	5.562	0.000	0.000	1.000
SIH4	2	207.6	4.084	0.000	0.000	1.000
SIHF3	2	180.8	4.681	0.000	0.000	1.000
SO	1	301.000	3.993	0.000	0.000	1.000
SO2	2	252.000	4.290	0.000	0.000	1.000
SO3	2	378.400	4.175	0.000	0.000	1.000
TMG	2	378.2	5.52	0.000	0.000	1.000



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## Chapter 6: Description and Properties of Particles

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Use of Particle Tracking to determine particle size distributions in a gas-particle flow requires identification of a condensed-phase material that may exist in a form that is dispersed within the gas-flow. In addition, you must specify certain properties of the particle “cloud” that will be tracked. This section describes the necessary input to the chemistry-set files, which are needed to establish these properties. Further discussions, of how kinetics rates may be specified to control the particle nucleation, growth, and transformation, are available in Chapter [Particle Size-Distribution Tracking](#) of the [Chemkin-Pro Theory Manual](#) .

Examples are available in the ANSYS Chemkin-Pro Tutorials Manual to illustrate how required information is presented to the Particle Tracking feature.

### 6.1. Description and Properties of the Particle Material

---

#### 6.1.1. Dispersed Material

Within a reactor model that enables Particle Tracking, the simulation treats a particle population as a collection of tiny solid or liquid material pieces suspended in bulk gas. This dispersed material concept represents the fact that particles are in a condensed phase and also allows use of existing surface-kinetics capabilities to handle gas-particle interactions.

Since the particles represent a condensed-phase material, all particle-related definitions are included in the surface chemistry input file. To declare a dispersed material, the Surface Kinetics keyword `MATERIAL` must be provided at the top of the Surface Kinetics Input file. This allows assignment of a name to the surface material. This material can then be designated as a dispersed material (i.e., it will be tracked in particle form), using the keyword `DISPERSED` that follows the `MATERIAL` statement. For example,

**Figure 6.1: Example of Dispersed Material Declaration**

```
MATERIAL soot
DISPERSED
END
```

With this entry, the material “soot” will be recognized by ANSYS Chemkin-Pro as a dispersed material. Note that an `END` keyword is needed to close the `DISPERSED` keyword block, although at this time there is no additional information included in the block.

It is possible to have more than one type of particle co-exist in the same system, although currently the Particle Tracking equations do not consider interactions between different types of particles. Different types of particles are defined as different dispersed materials. Definitions of multiple dispersed or non-dispersed materials are separated by the `MATERIAL` keywords. For example, if a chemical system contains two types of particles, such that one is called soot and the other is called silicon, they should be declared in two separate `MATERIAL` blocks as illustrated in [Figure 6.2: Example of Two Material Blocks \(p. 96\)](#) .

**Figure 6.2: Example of Two Material Blocks**

```

MATERIAL soot
DISPERSED
END
REACTIONS
...
END
MATERIAL silicon
DISPERSED
END
REACTIONS
...
END

```

### 6.1.2. Particle Composition

One of the properties differentiating one type of particle from another is the chemical composition of the particle. The chemical composition of the particles is determined by the chemical composition of the sole bulk species specified for the dispersed material. There can only be one bulk species specified. This determines the “chemical unit” of the particle and this “chemical unit” for the initially formed condensed “species” in the material. This “chemical unit” can be a single atom, a group of atoms, or a chemical compound. ANSYS Chemkin-Pro identifies the “chemical unit” of the particle by the sole bulk species on the dispersed material. For example, [Figure 6.3: Dispersed Graphite Material Declaration With Chemical Composition \(p. 96\)](#) defines a particle type called “soot”.

**Figure 6.3: Dispersed Graphite Material Declaration With Chemical Composition**

```

MATERIAL soot
DISPERSED
END
BULK/GRAPHITE/ C(B) /1.8/
END
THERMO
C(B)          121286C    1          S  0300.00   5000.00  1000.00      1
0.14901664E+01 0.16621256E-02-0.06687204E-05 0.12908796E-09-0.09205334E-13  2
-0.07074018E+04-0.08717785E+02-0.06705661E+01 0.07181499E-01-0.05632921E-04  3
0.02142298E-07-0.04168562E-11-0.07339498E+03 0.02601595E+02      4
END
REACTIONS
...
END

```

The BULK declaration line indicates that the core of the “soot” particles consists of units of bulk species C(B) and the bulk density  $\rho_B$  of the particle core is 1.8 [gm/cm<sup>3</sup>]. The actual chemical composition of C(B), the core of the “soot” particle, is a single carbon atom as it is defined in the Thermodynamic Data section that follows the BULK declaration.

Another example is given in [Figure 6.4: Dispersed Silicon Dioxide Material Declaration With Chemical Composition \(p. 96\)](#), for a compound particle composed of silicon dioxide.

**Figure 6.4: Dispersed Silicon Dioxide Material Declaration With Chemical Composition**

```

MATERIAL silicon
DISPERSED
END
BULK/OXIDE/ SiO2(B) /2.533/
END
THERMO

```



```

SIO2(B)          72391SI  10   2           S    298.00   2000.00 1000.00   1
 0.48925619E+01  0.41191629E-02-0.94570083E-07-0.80073115E-09 0.25433412E-12  2
-0.11005530E+06-0.23469570E+02 0.22325585E+01 0.12478522E-01-0.28715690E-05  3
-0.96847970E-08 0.62160411E-11-0.10962063E+06-0.10594849E+02  4
END
REACTIONS
...
END

```

### 6.1.3. Particle Class

Since the Particle Tracking feature employs the method of moments to solve the size distribution, it is important to understand the concept of particle class and how this class concept is connected to surface reactions that describe particle nucleation and mass growth. We define the class of a particle by the number of bulk species in its core. The “soot” particle declared in [Figure 6.4: Dispersed Silicon Dioxide Material Declaration With Chemical Composition \(p. 96\)](#) provides an example. A “soot” particle of class 100 has a core consisting of 100 C(B) species regardless of whether or not other species and atoms might exist on the surface of the particle.

When a particle nucleus is created from gas-phase precursors, its class, that is, the inception class, is determined by the stoichiometric coefficient of the bulk species in the nucleation reaction. For example, the nucleation reaction in [Figure 6.5: Nucleation Reaction Creating Particle Nuclei of Class 32 \(p. 97\)](#) creates particle nuclei of class 32:

**Figure 6.5: Nucleation Reaction Creating Particle Nuclei of Class 32**

```

2A4 => 32C(B) + 20 H(se) + 28.72 open(se)      1.0E10   0.5   0.0
          NUCL

```

The syntax of the nucleation reaction will be discussed in a later section. A surface reaction resulting in a net gain in the number of bulk species increases the size of the particle and vice-versa.

### 6.1.4. Mass and Volume of an Individual Particle

The mass of a particle is computed by summing the masses of all bulk species molecules in the core. According to the particle class definition, the mass of a class  $j$  particle becomes

$$m_p(j) = j \times m_0 \quad (6.1)$$

The mass of a single bulk species molecule  $m_0$  is assumed to be constant and can be calculated from

$$m_0 = W_B / N_{avo} \quad (6.2)$$

where  $W_B$  is the molar weight of the bulk species and  $N_{avo} = 6.022 \times 10^{23} [\text{mole}^{-1}]$  is the Avogadro number. The volume of a class  $j$  particle can be calculated from its mass and bulk density of the particle core as

$$V_p(j) = m_p(j) / \rho_B = j \times m_0 / \rho_B \quad (6.3)$$

The bulk density of the particle core  $\rho_B$  has implicitly accounted for the effect of molecule packing inside the core and its value is given when the bulk species is declared. It thus can be seen that both particle mass and volume are proportional to its class. Up to this point, there is no assumption regarding the shape of the particles so [Equation 6.1 \(p. 97\)](#) to [Equation 6.3 \(p. 97\)](#) are generally applicable to particles of all shapes.

### 6.1.5. Diameter and Surface Area of an Individual Particle

However, in order to derive a characteristic length scale of a particle, it is necessary to make assumption about its geometric shape. Currently, we assume that all particles are spherical. Accordingly, the representative diameter of a class  $j$  particle can be written as

$$d_p(j) = d_j = \left( \frac{6}{\pi} \times V_p(j) \right)^{1/3} = \left( \frac{6m_0}{\pi\rho_B} \right)^{1/3} j^{1/3} = d_0 \times j^{1/3} \quad (6.4)$$

The sphere-equivalent surface area of a class  $j$  particle is then given as

$$A_{s,p}(j) = \pi d_p^2(j) = \pi d_0^2 \times j^{2/3} = A_{s,0} \times j^{2/3} \quad (6.5)$$

In the above equations,

$$d_0 = \left( \frac{6m_0}{\pi\rho_B} \right)^{1/3} \quad (6.6)$$

and

$$A_{s,0} = \pi d_0^2 \quad (6.7)$$

are respectively the “unit” diameter and the “unit” surface area of the bulk species in particle core.

---

## Chapter 7: Using the FITDAT Utility

---

FITDAT is a utility that produces the polynomial fitting coefficients required as input for each species defined in a Gas-phase Kinetics or Surface Kinetics input file. The program accepts a molecule description in the form of character-string keywords, followed by thermodynamic data in a variety of formats. It then performs a least-squares fitting procedure for thermodynamic data, and writes an output file (e.g. *fitdat.out*) that contains the fit results and information about the quality of the fit. The file may also contain error diagnostics. The default format for the fit results is polynomial fitting coefficients for each of two temperature-ranges, as expected by the Gas-phase Kinetics and Surface Kinetics Pre-processors. An optional output format is also available if more than two temperature-ranges are desired.

Details of the various input formats for the thermodynamic data are described in [FITDAT Examples \(p. 105\)](#). The first option is to input a table of specific heat, enthalpy, and entropy values as functions of temperature. Several formats are accepted, corresponding to those used by standard references for thermodynamic data. The second option is to input thermodynamic data in the form of polynomial fitting coefficients, which *FITDAT* will convert to the format used by ANSYS Chemkin-Pro. Again, several formats are accepted, corresponding to those used by standard compilations of thermodynamic data. The third option is to input the molecule's standard enthalpy, standard entropy, and vibrational frequencies, which are then used to estimate the thermodynamic properties.

The fit results can be cut and pasted directly into a thermodynamics data file, or a *Gas-phase Kinetics* or *Surface Kinetics* input file for use with ANSYS Chemkin-Pro. In addition to this output, *FITDAT* creates file(s) named *species\_name.csv* (e.g. *H2.csv*) containing a table of comma-delimited data for each input species. These files facilitate visualization of evaluated fit results compared to the user's input data.

### 7.1. Running *FITDAT* from the User Interface

---

In the ANSYS Chemkin-Pro Interface, *FITDAT* is run from the Utility menu. To open the *FITDAT* panel, select the **Utility > Run 'FitDat' Polynomial Equation Fitting Utility...** menu option. The panel shown in [Figure 7.1: Utilities—'Fitdat' Polynomial Equation Fitter \(p. 100\)](#) will be displayed in the Working Area of the User Interface.

**Figure 7.1: Utilities—'Fitdat' Polynomial Equation Fitter**

The user must first assemble an input file that describes the fitting operation desired for the *FITDAT* session. The syntax of that input file is described in [Keyword Syntax and Rules \(p. 101\)](#) . Once the input file is assembled, *FITDAT* can be run by completing the following steps:

1. Use the **Working Dir** browse or pull-down menu tools to select a working directory. This is the directory where output files from the *FITDAT* run will be created.
2. Use the **Input File** browse or pull-down menu tools to select an input file. The syntax of the input file is described in [Keyword Syntax and Rules \(p. 101\)](#) .
3. Select an **Output File** name. Type a new name in the text box if you want to modify it from the default.
4. Use the **Run FitDat** button to execute the *FITDAT* utility.
5. Use the **View Results** button to examine the output file.
6. The user can import a *FITDAT species\_name.csv* file into the ANSYS Chemkin-Pro Post-Processor to plot the fitting results. For more information about the Post-Processor, see the new [Chemkin-Pro Visualization Manual](#) .

## 7.2. Programming with FITDAT

The *FITDAT* Utility is written as a FORTRAN subroutine that is called from a driver routine, and is part of the ANSYS Chemkin-Pro library. We provide both C++ and FORTRAN driver routines. The driver routine performs the function of allocating total memory usage through definition of array sizes, as well as opening input and output files. *FITDAT* checks internally to ensure that the allocated work arrays are sufficiently large to process the input data. Users modifying the programs should be experienced with compiling and linking program files on their operating system and must have either a C++ or FORTRAN compiler installed.

## 7.3. Keyword Syntax and Rules

The *FITDAT* Utility input is in a Keyword format. On each input line, an identifying Keyword must appear first. For some Keywords only the Keyword itself is required, while for others, additional information is required. The order of the Keyword input is generally unimportant. The rules governing the syntax of the Keyword images are listed below:

**Table 7.1: Summary of Rules for Keywords**

Rule	Description
1	The first character-string in the line must be a keyword; the length of the character-string depends on keyword descriptions.
2	Any further input associated with the keyword can appear anywhere after the keyword, through column 100. The specific starting column is not important, as long as there is at least one space after the keyword.
3	When more than one piece of information is required, the order in which the information appears is unimportant.
4	When numbers are required as input, they may be stated in either integer, floating point, or scientific "E" format. The utility converts the numbers to the proper type. The double precision specifier is not recognized; however, conversion to double precision is done internally as necessary.
5	When more than one piece of information is required, the pieces are delimited by one or more blank spaces.

## 7.4. FITDAT Keywords

**Table 7.2: FITDAT Keywords**

Keyword	Definition			
SPEC	A species character-string symbol, to be used in the thermodynamic data and in an ANSYS Chemkin-Pro reaction mechanism, and in the name of the post-processing data file.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Species</i>	Required	--	SPEC <b>OH</b>
	<b>Keyword Usage</b>	Optional keyword. By default, this keyword is not used unless it can be determined from the data source.		
ELEM	The elemental composition of the species.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Element</i>	Required	--	ELEM <b>O 1</b>  ELEM <b>H1</b>
	<i>Number of elements</i>	Required	--	ELEM <b>O 1</b>  ELEM <b>H 1</b>
	<b>Keyword Usage</b>	Optional keyword. By default, this keyword is not used unless it can be determined from the data source		

Keyword	Definition			
DIAG	The level of fitting procedure diagnostics printed to the output file. DIAG or DIAG 1 will print a summary of data vs. polynomial evaluation relative errors. DIAG 2 will print tables of input table vs. polynomial evaluations, as well as the summary of relative error.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Diagnostic level</i>	Optional	--	DIAG <b>2</b>
	<b>Keyword Usage</b>	Optional keyword. By default, no diagnostics are printed.		
NOTE	Print a 6-character legend to columns 19-24 of the output thermodynamic data. For example, NOTE 101602 notes the date of October 16, 2002, while NOTE Jan888 notes a JANAF data source.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Legend</i>	Required	--	NOTE <b>101602</b>  NOTE <b>Jan888</b>
	<b>Keyword Usage</b>	Optional keyword. By default, no notes are printed.		
PHAS	The phase of the species, G (gas), L (liquid), or S (solid).			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Phase</i>	Required	--	PHAS <b>G</b>
	<b>Keyword Usage</b>	Optional keyword. By default, the phase G is used unless it can be determined from data source.		
LINR	The linearity of the molecule; Y (molecule is linear) or N (no).			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Linearity</i>	Required	--	LINR <b>Y</b>
	<b>Keyword Usage</b>	Optional keyword. By default, this keyword is not used unless it can be determined from the data source.		
TMIN	The minimum temperature requirement for the polynomial; if TMIN is lower than the starting temperature of input data, thermodynamic properties will be extrapolated at this point.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Temperature</i>	Required	K	TMIN <b>300</b>
	<b>Keyword Usage</b>	Optional keyword. By default, the minimum temperature is 300 K unless it can be determined from data source.		
TMAX	The maximum temperature requirement for the polynomial; if TMAX is greater than the ending temperature of input data, thermodynamic properties will be extrapolated at this point.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Temperature</i>	Required	K	TMAX <b>5000</b>

Keyword	Definition			
	<b>Keyword Usage</b>	Optional keyword. By default, the maximum temperature is 5000 K unless it can be determined from data source.		
TEMP	One or more temperatures dividing the ranges of the polynomial, at which the functional values are constrained; all TEMP values must be between TMIN and TMAX. Each TEMP given will result in a set of polynomial coefficients. If no TEMP is given, there will be one set of coefficients.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Temperature or temperature range</i>	Required	K	TEMP <b>1500</b>  TEMP <b>1000 2000</b>
	<b>Keyword Usage</b>	Optional keyword. By default, this keyword is not used unless it can be determined from the data source.		
H298	Species' formation enthalpy at 298.15 K.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Enthalpy</i>	Required	kcal/mole	H298 <b>9.32</b>
	<b>Keyword Usage</b>	Optional keyword. By default, this keyword is not used unless it can be determined from the data source.		
NO298	Indicates that the <i>FITDAT</i> program should not try to constrain the species' formation enthalpy at the 298.15 K value. Normally the <i>FITDAT</i> program will attempt to exactly match the temperature fit at the 298.15 K point, but in some cases (e.g., the data point is not available) it may be desirable to remove this constraint.			
	Parameters	Optional/Reqd.	Units	Examples
		--	--	NO298
	<b>Keyword Usage</b>	Optional keyword. By default, the fit is constrained to exactly match the input value at 298.15 K.		
S298	Species' formation entropy at 298.15 K.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Entropy</i>	Required	cal/mole	S298 <b>43.88</b>
	<b>Keyword Usage</b>	Optional keyword. By default, this keyword is not used unless it can be determined from the data source.		
DATA	A table of data will follow, the format and contents of which depends on the data type given with this keyword.			
	Parameters	Optional/Reqd.	Calorie-based Units	Examples
	<i>Type of data table</i>	Required	--	DATA <b>CHEM</b>  DATA <b>JANAF</b>  DATA <b>NIST</b>

Keyword	Definition			
				DATA <b>NASA</b>
	<b>Keyword Usage</b>	Optional keyword. By default, the DATA CHEM option is used.		
POLY	A set of polynomial data will follow, the format and contents of which depends on the polynomial type given with this keyword. The CHEM option will display ANSYS Chemkin-Pro-formatted polynomial records. The SHOM option will display Shomate polynomial records. The NASA option will display NASA-formatted polynomial records.			
	Parameters	Optional/Reqd.	Calorie-based Units	Examples
	<i>Set of polynomial data</i>	Required	--	POLY <b>CHEM</b>  POLY <b>SHOM</b>  POLY <b>NASA</b>
	<b>Keyword Usage</b>	Optional keyword. By default, the POLY CHEM option is used.		
VIBE	One or more species' vibrational frequency.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Vibrational frequency</i>	Required	cm <sup>-1</sup>	VIBE 999.83
	<b>Keyword Usage</b>	Optional keyword.		
NPTS	Number of points to generate from TMIN to TMAX, when evaluating properties data from POLY or VIBE.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Number of points</i>	Required	--	NPTS <b>50</b>
	<b>Keyword Usage</b>	Optional keyword. By default, 100 points are generated.		
DELT	Temperature increment used from TMIN to TMAX, when evaluating properties data from POLY or VIBE.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Temperature</i>	Required	K	DELT <b>50</b>
	<b>Keyword Usage</b>	Optional keyword. By default, DELT value depends on the NPTS value.		
END	End of input, and start of the fitting process for the current species.			
	<b>Keyword Usage</b>	Required keyword.		



## 7.5. FITDAT Examples

This section discusses input files that allow *FITDAT* to provide thermodynamic data fitting coefficients using several different methods. These examples show NIST, Shomate, NASA, and other data formats ([DATA CHEM Input Format \(p. 105\)](#) through [VIBE Input Format \(p. 109\)](#) ).

*FITDAT* is run from the ANSYS Chemkin-Pro Interface by selecting it from the **Utility** menu (see [FITDAT Utility for Fitting Polynomials to Thermodynamic Data](#) for more information). After running *FITDAT*, users may then launch the Chemkin-Pro Post-Processor using the **View > Graphical Post-processor** menu option. This action will actually result in a warning message and the display of a "Sample Plot"; as *FITDAT* does not produce a typical solution file like other Chemkin-Pro problem and *FITDAT* results will therefore need to be plotted using the Import option in the Chemkin-Pro Post-Processor. The user selects the Import option from the Post-Processor's File menu. This opens a file browser to allow the user to select a *species\_name.csv* file for plotting of fit results. After the file has been selected, further select the following items from the Select the Import File Format dialog: **Comma** radio button, Skip 2 lines of text (**Skip** slider control), and **Read column titles** check box.

### 7.5.1. DATA CHEM Input Format

This is an example of the minimum input required to fit default type of data, which is four columns consisting of temperature (K), and species properties  $C_p$  (cal/mole-K),  $S$  (cal/mole-K), and  $H(T) - H(298)$  (kcal/mole). Defaults are PHAS=G, TMIN=300, and TMAX=5000, the first and last positive data points, but keywords may be used to supersede these values.

**Figure 7.2: DATA CHEM Input File**

```
SPEC OH
ELEM O 1
ELEM H 1
H298 9.32
TEMP 1500
DATA
0300.00 007.165 043.926 000.013
0400.00 007.087 045.974 000.725
:
4900.00 009.232 065.778 038.571
5000.00 009.249 065.965 039.495
END
```

### 7.5.2. POLY CHEM Input Format

This is an example of the minimum input required to fit data evaluated from an existing ANSYS Chemkin-Pro -format polynomial; defaults SPEC=OH, ELEM, PHAS=G, TMIN=300, TMAX=5000, and TEMP=1000 are obtained from the polynomial, and H298 by an evaluation of the polynomial, but keywords may be used to supersede these values. This option might be used to generate fits for a different temperature range where the original data are no longer available.

**Figure 7.3: POLY CHEM Input File**

```
POLY CHEM
OH 1212860 1H 1 G 0300.00 5000.00 1000.00 1
0.02882730E+02 0.10139743E-02-0.02276877E-05 0.02174683E-09-0.05126305E-14 2
0.03886888E+05 0.05595712E+02 0.03637266E+02 0.01850910E-02-0.16761646E-05 3
0.02387202E-07-0.08431442E-11 0.03606781E+05 0.13588605E+01
END
```

*FITDAT* evaluates the ANSYS Chemkin-Pro polynomial as described in [Running \*FITDAT\* from the User Interface \(p. 99\)](#), to obtain thermodynamic properties for fitting. A table of NPTS temperatures from TMIN to TMAX will be used to evaluate the properties; keywords NPTS or DELT may be used to modify this phase.

### 7.5.3. DATA NIST Input Format

This is an example of the minimum input required to fit NIST-format data, which is 5 columns consisting of temperature (K), and species properties  $C_p$  (cal/mole·K),  $S$  (cal/mole·K),  $-(G^0 - H^0(298.15))/T$  (cal/mole·K) and  $H(T) - H(298)$  (kcal/mole). Input data can be obtained from the *NIST Chemistry WebBook*[8] (p. 345),<sup>p. 124</sup> using the following steps:

1. At the start of the NIST menu (<http://webbook.nist.gov/chemistry/form-ser.html>), choose **calorie-based units** in the toggle under question #3, when selecting the desired units for thermodynamic data.
2. Perform a **Formula Search** (e.g., search for OH).
3. Select **View Table** option under the Heat Capacity heading.
4. In the table view, highlight and copy the table text, then paste into a text file.

Defaults are PHAS=G, and TMIN=300, TMAX=6000, the first and last positive data points greater than 298, but keywords may be used to supersede these values.

**Figure 7.4: DATA NIST Input File**

```
SPEC OH
ELEM O 1
ELEM H 1
H298 9.318131
TEMP 1500.
DATA NIST
300. 7.16 43.95 43.91 0.01
400. 7.09 46.00 44.19 0.73
:
5900. 9.41 67.53 59.42 47.89
6000. 9.43 67.69 59.55 48.83
END
```

### 7.5.4. POLY SHOM Input Format

This is an example of the minimum input required to convert a Shomate polynomial to ANSYS Chemkin-Pro format; The Shomate equations are given in [Equation 7.1 \(p. 107\)](#) through [Equation 7.3 \(p. 107\)](#), where  $t = \text{Temperature(K)}/1000$ . Parameters (A, B, C, D, E, F, G, and  $H^0_f(298)$ ) can be obtained from the *NIST Chemistry WebBook*. [8] (p. 345)

1. At the start of the NIST menu (<http://webbook.nist.gov/chemistry/form-ser.html>), choose **calorie-based units** in the toggle under question #3, when selecting the desired units for thermodynamic data.
2. Perform a **Formula Search** (e.g., search for OH).
3. Highlight and copy the table of parameters (including the heading row and the rows for the A, B, C, D, E, F, G parameters), then paste these into a text file.

Defaults are PHAS=G, TMIN=298, TMAX=6000, and TEMP=1000 are obtained from the Shomate data, and H298 by an evaluation of the polynomial, but keywords may be used to supersede the defaults.

**Figure 7.5: POLY SHOM Input File**

```
SPEC OH
ELEM O 1
ELEM H 1
POLY SHOM
Temperature (K) 298. - 1300. 1300. - 6000.
A 7.714551 6.870701
B -2.715801 1.126790
C 3.251781 -0.194724
D -0.919332 0.013085
E -0.000319 -0.656747
F 7.110691 6.313191
G 53.91451 51.17510
END
```

$$C_p = A + Bt + Ct^2 + Dt^3 + \frac{E}{t^2} \quad (7.1)$$

$$H - H(298) = At + \frac{Bt^2}{2} + \frac{Ct^3}{3} + \frac{Et^4}{4} - \frac{E}{t} + F - H(298) \quad (7.2)$$

$$S = A \ln(t) + Bt + \frac{Ct^2}{2} + \frac{Dt^3}{3} - \frac{E}{2t^2} + G \quad (7.3)$$

A table of NPTS temperatures from TMIN to TMAX will be used to evaluate the properties; keywords NPTS or DELT may be used to modify this process.

### 7.5.5. DATA NASA Input Format

This is an example of the minimum input required to fit NASA-format data, which is at least four columns consisting of temperature (K), and species properties  $C_p$  (cal/mole-K),  $H(T) - H(298)$  (kcal/mole), and  $S$  (cal/mole-K). NASA data can be obtained from the Properties From Coefficients (PFC) [8] (p. 345) program; request **calorie-based units**, and highlight, copy, and paste the resulting table into a text file. Defaults are PHAS=G, TMIN=300, TMAX=6000, the first and last positive data points, and H298 is the column 6 value at T=298.15, but keywords may be used to supersede the defaults.

**Figure 7.6: DATA NASA Input File**

```
SPEC OH
ELEM O 1
ELEM H 1
DATA NASA
! THERMODYNAMIC FUNCTIONS CALCULATED FROM COEFFICIENTS FOR OH
! T Cp H-H298 S -(G-H298)/T H delta Hf log K
! deg-K cal/mol-K kcal/mol cal/mol-K cal/mol-K kcal/mol kcal/mol
0 0. -2.106 0. INFINITE 6.803 8.853 INFINITE
200 7.293 -0.707 41.035 44.572 8.202 8.877 -8.9035
298.15 7.143 0.000 43.915 43.915 8.910
:
:
5900 9.620 48.463 67.672 59.458 57.373 6.636 0.3749
6000 9.625 49.425 67.834 59.596 58.335 6.573 0.3790
END
```

## 7.5.6. POLY NASA Input Format

This is an example of the minimum input required to convert a NASA polynomial[9] (p. 345) to Chemkin-Pro format. The equations defining polynomials are given in Equation 7.4 (p. 108) through Equation 7.6 (p. 108). NASA polynomial data can be obtained from the Properties From Coefficients (PFC)[10] (p. 345)<sup>p. 124</sup> and then highlighted, copied, and pasted into a text file. Defaults for SPEC, ELEM, PHAS, TMIN, TMAX, TEMP, and H298 are obtained from the polynomial, but may be superseded by keyword usage.

**Figure 7.7: POLY NASA Input File**

```
POLY NASA
OH          D0(H-OH): Ruscic,2002. Gurvich,1978 pt1 p110 pt2 p37.
 3 g 4/02 O   1.00H   1.00   0.00   0.00   0.00 0   17.00734   37278.206
 200.000 1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0   8813.106
-1.998858990E+03 9.300136160E+01 3.050854229E+00 1.529529288E-03-3.157890998E-06
 3.315446180E-09-1.138762683E-12 0.000000000E+00 2.991214235E+03 4.674110790E+00
 1000.000 6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0   8813.106
 1.017393379E+06-2.509957276E+03 5.116547860E+00 1.305299930E-04-8.284322260E-08
 2.006475941E-11-1.556993656E-15 0.000000000E+00 2.019640206E+04-1.101282337E+01
 6000.000 20000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0   8813.106
 2.847234193E+08-1.859532612E+05 5.008240900E+01-5.142374980E-03 2.875536589E-07
-8.228817960E-12 9.567229020E-17 0.000000000E+00 1.468393908E+06-4.023555580E+02
END
```

**Figure 7.8: Format details for POLY NASA Input Files**

```
line 1:      OH is species name
line 2:      3 is the number of temperature ranges
              5 sets of elemental composition, that is, 'O 1.00' and 'H 1.00'
              0 in the next field indicates a gas
              17.00734 is the molecular weight
              37278.206 is H298 heat of formation, J/mol
line 3:      200-1000 is the first temperature range,
              7 is the number of Cp/R polynomial coefficients,
              -2,-1,0,1,2,3,4,0 are the T exponents for the coefficients,
              8813.106 is H(298)-H(0), J/mol
line 4:      a1 through a5 for temperatures 200-1000K
line 5:      a6 through a7 for temperatures 200-1000K, a8 (not used),
              integration constants b1, b2
lines 6-end: same as 3-5, for more temperature ranges
```

The resulting non-dimensional thermodynamic properties are

$$\frac{C_p}{R} = a_1 T^{-2} + a_2 T^{-1} + a_3 + a_4 T + a_5 T^2 + a_6 T^3 + a_7 T^4 \quad (7.4)$$

$$\frac{H}{RT} = -a_1 T^{-2} + a_2 T^{-1} \ln(T) + a_3 + \frac{a_4 T}{2} + \frac{a_5 T^2}{3} + \frac{a_6 T^3}{4} + \frac{a_7 T^4}{5} + \frac{b_1}{T} \quad (7.5)$$

$$\frac{S}{R} = -\frac{a_1 T^{-2}}{2} - a_2 T^{-1} + a_3 \ln(T) + a_4 T + \frac{a_5 T^2}{2} + \frac{a_6 T^3}{3} + \frac{a_7 T^4}{4} + b_2 \quad (7.6)$$

A table of NPTS temperatures from TMIN to TMAX will be used to evaluate the properties; keywords NPTS or DELT may be used to modify this process.

## 7.5.7. DATA JANAF Input Format

This is an example of the minimum input required to fit JANAF-format data, which is at least five columns consisting of temperature (K), and species properties  $C_p$  (J/mole-K),  $S$  (J/mole-K),  $G$  (J/mole-



```

S298 49.4
TEMP 1000
VIBE 999.83
VIBE 2011.69
VIBE 2001.72
END

```

### 7.5.9. Example *FITDAT* Outputs

Figure 7.11: Example *fitdat.out* file (p. 110) shows the *fitdat.out* file that will be created if the DATA CHEM input file discussed in DATA CHEM Input Format (p. 105) is run through the *FITDAT* utility.

**Figure 7.11: Example *fitdat.out* file**

```

*****
*                               CHEMKIN Release 4.0                               *
*                               FITDAT Application                               *
*                               Thermodynamic properties fitting program.         *
* Copyright 1997-2002 Reaction Design. All Rights Reserved. *
*****

      WORKING SPACE REQUIREMENTS
      PROVIDED      REQUIRED
INTEGER          112          112
REAL             9534         9534

Reading keyword data...
Setting SPEC name:              OH
Setting ELEM # 1:               O 1
Setting ELEM # 2:               H 1
Setting H298:                   9.320E+00 Kcal/mole
Setting TEMP # 1:               1.000E+03 K
End of keyword input for species OH

Species OH Fit:
OH          O 1H 1      G 300.000 5000.000 1000.00      1
0.29446142E+01 0.91447172E-03-0.17338418E-06 0.95183610E-11 0.46042672E-15      2
0.38598718E+04 0.52419727E+01 0.35069641E+01 0.12114174E-02-0.44383205E-05      3
0.53991545E-08-0.19835349E-11 0.36200845E+04 0.18923732E+01      4

Reading keyword data...
End of input file...

```

Figure 7.12: Example *fitdat.out* file with more than two temperature ranges (p. 110) shows example output that would result if the input discussed in DATA CHEM Input Format (p. 105) is modified to include polynomial coefficients for more than two temperature ranges (e.g., adding keyword line: TEMP 2500).

**Figure 7.12: Example *fitdat.out* file with more than two temperature ranges**

```

*****
*                               CHEMKIN Release 4.0                               *
*                               FITDAT Application                               *
*                               Thermodynamic properties fitting program.         *
* Copyright 1997-2002 Reaction Design. All Rights Reserved. *
*****

```

```

      WORKING SPACE REQUIREMENTS
      PROVIDED      REQUIRED
INTEGER      112      112
REAL         9534     9534

```

Reading keyword data...

```

Setting SPEC name:      OH
Setting ELEM #  1:      O   1
Setting ELEM #  2:      H   1
Setting H298:           9.320E+00 Kcal/mole
Setting TEMP #  1:      1.000E+03 K
Setting TEMP #  2:      2.500E+03 K
End of keyword input for species OH

```

Species OH Fit:

```

OH          O   1H   1          G   300.000  5000.000          1
TEMP   300.000  1000.000  2500.000  5000.000
0.31521126E+01 0.77090695E-03-0.15393767E-06 0.13363294E-10-0.27768811E-15
0.36675921E+04 0.39045946E+01
0.34408417E+01-0.28167277E-03 0.83197801E-06-0.34404565E-09 0.44913015E-13
0.37077941E+04 0.26162167E+01
0.37729215E+01-0.61576963E-03-0.15821000E-06 0.13103019E-08-0.61722943E-12
0.35916670E+04 0.76556823E+00

```

Reading keyword data...

End of input file...





---

## Chapter 8: CHEMKIN Project Input: Keyword Syntax and Rules

---

In most cases, a Reactor Model input file is written by the ANSYS Chemkin-Pro Interface before a simulation run based on the Chemkin-Pro Project Input. The panel context and “bubble” help within the Interface provide basic guidance for setting up model-specific input parameters. However, in some cases users may want further information about a model parameter usage and in other cases they may want to assemble their own input files outside of the User Interface. For such cases, this chapter together with [Reference Guide to Project Input Keywords \(p. 115\)](#) and [Alphabetical Listing of Project Input Keywords \(p. 123\)](#) contain detailed information about input options for each Reactor Model. This chapter provides an overview of the syntax and rules for such parameter input.

User input information is generally written to a Reactor Model input file in “keyword” format. In this format, each input line starts with an identifying keyword. For some input, only the keyword itself is required, while others require one or more pieces of additional information. Many keywords have default values associated with them. If these default values are appropriate for the user’s problem, then these keywords do not need to be included in the input file. In the case of restarts or continuation problems, some of the parameters can be changed from what was used in the previous solution. If these keywords are not included or not changed in the input keyword list for continuations or restarts, then the parameters will retain their former values. In the list of keywords that follow, we indicate whether or not each keyword may be changed on a restart from a previous solution. The order of the keyword input is not important. The general rules governing the syntax of the keyword lines are listed in [Table 8.1: Summary of the Rules for Keywords \(p. 113\)](#).

---

### Note:

Note that you can turn on or off the display of the “Keyword” associated with an ANSYS Chemkin-Pro Interface input parameter, using the modal option in the Preferences panel.

---

**Table 8.1: Summary of the Rules for Keywords**

Rule	Description
1	The first character-string in the line must be a keyword; the length of the character-string depends on keyword descriptions.
2	Any further input associated with the keyword can appear anywhere after the keyword, through column 80. The specific starting column is not important, as long as there is at least one space after the keyword.
3	When more than one piece of information is required, the order in which the information appears is important.
4	When numbers are required as input, they may be stated in integer, floating-point, or “E” format. ANSYS Chemkin-Pro converts the numbers to the proper type internally. The double precision specification D is not recognized; however, the double precision conversion will be done internally, as necessary.
5	When species names are required as input, they must appear exactly as they are specified in the <i>Gas-phase Kinetics</i> and <i>Surface Kinetics</i> input files.

Rule	Description
6	When more than one piece of information is required, the pieces are delimited by one or more blank spaces.
7	If contradictory or duplicate keywords are input, ANSYS Chemkin-Pro uses the information that is last read. Under some circumstances, this will result in a warning printed to the output file.
8	A "comment" line is one that has either a period (.), slash (/), or exclamation mark (!) as the first non-blank character. In addition, on any Keyword line, any input that follows an exclamation mark is taken as a comment. All input lines, including comments, are printed to the output.
9	The keyword <code>END</code> must be the last input card. <code>END</code> keywords are required between sets of parameters for continuations.
10	If no parameter is given, then the keyword stands alone on the input line; keywords with parameters are demonstrated with examples.

---

## Chapter 9: Reference Guide to Project Input Keywords

---

In this chapter, we group the available input reactor project input options (keywords) according to the Reactor Model with which they may be used. Note that many keywords can be used with several different Reactor Models and that there are a few cases where keywords that share the same name may have different meanings for different Reactor Models. General information about keyword syntax and rules is given in [CHEMKIN Project Input: Keyword Syntax and Rules \(p. 113\)](#). A detailed, alphabetical listing of all keywords is given in [Alphabetical Listing of Project Input Keywords \(p. 123\)](#). This chapter is meant to serve as a quick cross-reference to the more detailed information in [Alphabetical Listing of Project Input Keywords \(p. 123\)](#).

### 9.1. Closed 0-D Reactor Models

---

#### 9.1.1. Internal Combustion HCCI Engine

The following keywords can be used to build an input file for an IC HCCI Engine Reactor Model:

ADAP, ADD, AEXT, AGGA, AGGB, AGGD, AGGE, AGGFD, AGGMN, AROP, ASEN, ASTEPS, ATLS, ATOL, AVALUE, AVAR, BETA, CAATQ, CKTRN, CLSC, CLSM, CMPR, CNTN, CNNT, COLR, CYBAR, DEGO, DELT, DIST, DTDEG, DTIGN, DTSV, EGRR, END, EPSR, EPSS, EPST, EQUI, FUEL, FVCP, GFAC, GMHTC, GVEL, HIMP, HTC, HTCPR, ICEN, ICHF, ICHH, ICHT, ICHW, IPSR, KLIM, LODR, LOLR, MAXIT, MCUT, MMASS, NADAP, NCANG, NEWRUN, NMOM, NNEG, NOCG, NREV, NSOL, OXID, PNDE, PRDL, PRES, PRNT, PROE, PSBAR, PTM\_SECTION\_SIZEDEP\_A0, PTM\_SECTION\_SIZEDEP\_COLEFF, PTM\_SECTION\_SIZEDEP\_DSTAR, PTM\_SECTION\_SIZEDEP\_HAMAKER, PTM\_SECTION\_USERBULKROP, PTM\_SECTIONAL, PVFE, PVS0, PVSIN, PVST, QEXP, QFUN, QLOS, QPRO, QRGEQ, REAC, RELAXC, RLGAS, RLMIX, ROP, RPM, RSTR, RTLS, RTOL, SCLM, SCLS,, SENT, SIZE, SOLUTION\_TECHNIQUE, SSTT, STPT, SVS0, SVSS, SVST, TEMP, TEXP, TIFP, TIME, TLIM, TRAN, TRES, TRST, TSTR, TTIM, UIGN, UREF, USET, VOLC, VOLD, WENG, WOSP1, WOSP2, WOSP3, XMLI

#### 9.1.2. Closed Homogeneous Batch Reactor

The following keywords can be used to build an input file for a Closed Homogeneous Reactor Model:

ADAP, ADD, AEXT, AFRA, AGGA, AGGB, AGGD, AGGE, AGGFD, AGGMN, AINT, AREA, AREAQ, AROP, ASEN, ASTEPS, ATLS, ATOL, AVALUE, AVAR, BETA, BLKEQ, BULK, CLSC, CLSM, CNTN, CNNT, COLR, CONP, CONV, COTV, DELT, DIST, DTIGN, DTSV, EGRR, END, ENRG, EPSG, EPSR, EPSS, EPST, EQUI, ETCH, FUEL, GFAC, GMHTC, HTC, HTRN, IPSR, IRET, ISTP, KLIM, MAXIT, MCUT, MMASS, NADAP, NEWRUN, NMOM, NNEG, NOCG, NSOL, OXID, PBDEN, PNDE, PPRO, PRES, PRNT, PROE, PTM\_SECTION\_SIZEDEP\_A0, PTM\_SECTION\_SIZEDEP\_COLEFF, PTM\_SECTION\_SIZEDEP\_DSTAR, PTM\_SECTION\_SIZEDEP\_HAMAKER, PTM\_SECTION\_USERBULKROP, PTM\_SECTIONAL, PVFE, QFUN, QLOS, QPRO, QRGEQ, QRSEQ, REAC, RELAXC, RLGAS, RLMIX, ROP, RSTR, RTLS, RTOL, SCLM, SCLS, SCOR, SENG, SENT, SFAC, SIZE, SOLUTION\_TECHNIQUE, SSTT, STPT, SURF, TAMB, TEMP, TGIV, TIFP, TIME, TLIM, TPRO, TRAN, TRES, TRST, TSTR, TSTR, TTIM, UIGN, USET, VOL, VPRO, VTIM, WENG, XMLI

### 9.1.3. Closed Partially Stirred Reactor

The following keywords can be used to build an input file for a Closed PaSR Reactor Model:

ADAM, ATOL, BDF, CFL, CHEM, CLSE, CMIX, CTOL, CURL, DASP, DT, DT0, DTMX (transient), DTSV, END, EQUI, IEM, INIT, KOUT, MAXIT, MAXTIME, MIX, MIXT, NCFIT, NDPR, NNEG, NOJC, NPAR, PDF, PRES, QRGEQ, QRSEQ, RELAXC, RLGAS, RLMIX, RSTR, RTOL, SCAT, SIZE, SSMAXITER, TEMP, TIME, TRES, TRMAXITER, VOL, VPRO, WELL

### 9.1.4. Closed Plasma Reactor

The following keywords can be used to build an input file for a Closed Plasma Reactor Model:

ABSL, ADAP, AEXT, AFRA, AGGD, AGGE, AINT, AREA, AREAQ, AROP, ASEN, ASTEPS, ATIM, ATLM, ATLS, ATOL, AVALUE, AVAR, BETA, BLKEQ, BOHM, BPWR, BULK, CLSC, CLSM, CNTN, CNNT, CONP, COLR, CONV, DELT, DFAC, DIST, DTIGN, DTSV, ELSH, END, ENGE, ENRG, EPSG, EPSR, EPSS, EPST, ETCH, ETMP, GFAC, GMHTC, HTC, HTRN, IONE, IPSR, KLIM, MAXIT, MCUT, MMASS, NADAP, NEWRUN, NMOM, NNEG, NOCG, NSOL, PNDE, PPRO, PRES, PRNT, PROE, PVFE, PWRW, QFUN, QLOS, QLSE, QPRO, REAC, RELAXC, ROP, RSTR, RTIM, RTLM, RTLS, RTOL, SCLM, SCLS, SCOR, SENG, SENT, SFAC, SIZE, SOLUTION\_TECHNIQUE, SSTT, STPT, SURF, TAMB, TEBND, TEMP, TGIV, TIFP, TIME, TION, TLIM, TPRO, TRAN, TRES, TRST, TSTR, TTIM, USET, UIGN, VOL, VPRO, VTIM, WENG, WPRO, XMLI, XSDF, XSEK

### 9.1.5. Multi-Zone HCCI Engine Simulator

The following keywords can be used to build an input file for a Multi-Zone HCCI Engine Simulator:

ADAP, ADD, AEXT, AGGA, AGGB, AGGD, AGGE, AGGFD, AGGMN, AROP, ASEN, ASTEPS, ASWH, ATLS, ATOL, AVALUE, AVAR, BETA, CAATQ, CKTRN, CLSC, CLSM, CMPR, CNTN, CNNT, COLR, CYBAR, DEGO, DELT, DIST, DTDEG, DTIGN, DTSV, END, EPSR, EPSS, EPST, EQUI, FUEL, FVCP, GFAC, GMHTC, GVEL, HIMP, HTC, HTCPRO, ICEN, ICHF, ICHH, ICHT, ICHW, ICHT, IPSR, KLIM, LODR, LOLR, MAXIT, MCUT, MMASS, MQAFR, MZMAS, NADAP, NCANG, NEWRUN, NMOM, NNEG, NOCG, NREV, NSOL, NZONE, OXID, PNDE, PRDL, PRES, PRNT, PROE, PSBAR, PTM\_SECTION\_USERBULKROP, PTM\_SECTIONAL, PVFE, PVS0, PVSIN, PVST, QEXP, QFUN, QLOS, QPRO, QRGEQ, RELAXC, RLGAS, RLMIX, ROP, RPM, RSTR, RTLS, RTOL, SCLM, SCLS, SCOR, SENT, SIZE, SOLUTION\_TECHNIQUE, SSTT, STPT, TEMP, SVS0, SVSS, SVST, TEXP, TIFP, TIME, TLIM, TRAN, TRES, TRST, TSTR, TSWH, TTIM, UIGN, UREF, USET, VOL, VOLC, VOLD, WENG, WOSP1, WOSP2, WOSP3, XEST, XMLI, ZONEAVG

### 9.1.6. SI Engine Zonal Simulator

The following keywords can be used to build an input file for an SI Engine Zonal Simulator:

ADAP, ADD, AEXT, AGGA, AGGB, AGGD, AGGE, AGGFD, AGGMN, AROP, ASEN, ASTEPS, ASWH, ATLS, ATOL, AVALUE, AVAR, BETA, CAAC, CAATQ, CAEC, CASC, CKTRN, CLSC, CLSM, CMPR, CNTN, CNNT, COLR, CYBAR, DEGO, DEGE, DELT, DIST, DTDEG, DTIGN, DTSV, END, EPSR, EPSS, EPST, SIZE, EQUI, FUEL, FVCP, GFAC, GMHTC, GVEL, HSWC, HSWM, HSWT, HIMP, HTC, HTCPRO, ICEN, ICHF, ICHH, ICHT, ICHW, IPSR, KLIM, LODR, LOLR, MAXIT, MCUT, MMASS, NADAP, NCANG, NEWRUN, NMOM, NNEG, NOCG, NREV, NSOL, OXID, PNDE, PRDL, PRES, PRNT, PROE, PSBAR, PTM\_SECTION\_USERBULKROP, PTM\_SECTIONAL, PVFE, PVS0, PVSIN, PVST, QEXP, QFUN, QLOS, QPRO, QRGEQ, RELAXC, RLGAS, RLMIX, ROP, RPM, RSTR, RTLS, RTOL, SCLM, SCLS, SCOR, SENT, SIDR, SIKN, SIOA, SIZE, SOLUTION\_TECHNIQUE, SSTT, STPT, SVS0, SVSS, SVST, TEMP, TEXP, TIFP, TIME, TLIM, TRAN, TRES, TRST, TSTR, TTIM, UIGN, UREF, USET, VOL, VOLC, VOLD, WENG, WOSP1, WOSP2, WOSP3, XEST, XMLI, ZONEAVG

### 9.1.7. Direct Injection Diesel Engine Simulator

The following keywords can be used to build an input file for a Direct Injection Diesel Engine Simulator:

AFRFX, ATLRE, ATLTS, AZFAC, BTMIN, CAIR, DIEN, DINZL, FICA0, FIDUR, FILFY, FIMAS, FINJP, FINRD, FINTL, FITMP, FLINJ, LMLM, MVFAC, MXITS, NZCDC, NZDIA, NZHOL, NZINJ, NZLDR, NZRDR, NZRWL, QIAGE, TSFAC, TSTAU, VFFAC, VPARI, VPMOD

## 9.2. Open 0-D Reactor Models

### 9.2.1. Perfectly Stirred Reactor

The following keywords can be used to build an input file for a PSR Reactor Model:

ABFR, ABSL, AEXT, AFRA, AGGA, AGGB, AGGD, AGGE, AGGFD, AGGMN, AINT, AREA, AREAQ, AROP, ASEN, ASTEMS, ATIM, ATLM, ATLS, ATOL, AVALUE, AVAR, BETA, BLKEQ, BULK, CLSC, CLSM, CNTN, CNNT, COLR, CPROD, DELT, DFAC, DIST, DTIGN, DTMN, DTMX (steady-state), DTSV, EGRR, END, ENRG, EPSG, EPSR, EPSS, EPST, EQUI, ETCH, FLRT, FPRO, FUEL, GFAC, GMHTC, HTC, HTRN, INLET, IPSR, IRET, ISTP, KLIM, MAXIT, MAXTIME, MCUT, MMAX, NEWRUN, NJAC, NMOM, NNEG, NOCG, NOFT, NPSR, NSOL, OXID, PBDEN, PNDE, PNDI, PPRO, PRES, PRNT, PROD, PROE, PROI, PSURF, PTM\_SECTION\_SIZEDEP\_A0, PTM\_SECTION\_SIZEDEP\_COEFF, PTM\_SECTION\_SIZEDEP\_DSTAR, PTM\_SECTION\_SIZEDEP\_HAMAKER, PTM\_SECTION\_USERBULKROP, PTM\_SECTIONAL, PVFE, PVFI, QFUN, QLOS, QPRO, QRGEQ, QRSEQ, QXCO (p. 294), QXRA (p. 294), REAC, RECY, RELAXC, RELT, RLGS, RLMIX, ROP, RSTR, RTIM, RTLM, RTLS, RTOL, SCCM, SCCMPRO, SCLM, SCLS, SCOR, SENG, SENT, SFAC, SFLR, SIZE, SOLUTION\_TECHNIQUE, SPOS, SSMAXITER, SSTT, STPT, STST, SURF, TAMB, TAU, TEMP, TGIV, TIFP, TIM1, TIM2, TIME, TINL, TJAC, TLIM, TPRO, TRAN, TRES, TRMAXITER, TRST, TSCCM, TSTR, TTIM, UFAC, UIGN, USET, USEV (Restart), USEV (XMLI), USRIN, VOL, VPRO, VTIM, WENG, WPRO, XEST, XMLI, XMLS

### 9.2.2. Plasma Perfectly Stirred Reactor

The following keywords can be used to build an input file for a Plasma PSR Reactor Model:

ABSL, ADD, AEXT, AFRA, AGGA, AGGB, AGGD, AGGE, AGGFD, AGGMN, AINT, AREA, AREAQ, AROP, ASEN, ASTEMS, ATIM, ATLM, ATLS, ATOL, AVALUE, AVAR, BETA, BLKEQ, BOHM, BPWR, BULK, CLSC, CLSM, CNTN, CNNT, COLR, CPROD, DELT, DFAC, DIST, DTIGN, DTMN, DTMX (steady-state), DTSV, EGRR, ELSH, END, ENGE, EPSG, EPSR, EPSS, EPST, EQUI, ETCH, ETMP, FLRT, FPRO, FUEL, GFAC, GMHTC, HTC, HTRN, INLET, IONE, IPSR, IRET, ISTP, KLIM, MAXIT, MAXTIME, MCUT, MMAX, NEWRUN, NJAC, NMOM, NNEG, NOCG, NOFT, NPSR, NSOL, OXID, PNDE, PNDI, PPRO, PRES, PRNT, PROE, PROI, PSURF, PVFE, PVFI, PWRW, QFUN, QLSE, QPRO, QRGEQ, QRSEQ, QXCO (p. 294), QXRA (p. 294), REAC, RECY, RELAXC, RELT, ROP, RSTR, RTIM, RTLM, RTLS, RTOL, SCCM, SCCMPRO, SCLM, SCLS, SCOR, SENG, SENT, SFAC, SFLR, SIZE, SOLUTION\_TECHNIQUE, SPOS, SSMAXITER, SSTT, STPT, STST, SURF, TAMB, TAU, TEBND, TEIN, TEMP, TGIV, TIFP, TIM1, TIM2, TIME, TINL, TION, TJAC, TLIM, TPRO, TRAN, TRES, TRMAXITER, TRST, TSCCM, TSTR, TTIM, UFAC, UIGN, USET, USEV (Restart), USEV (XMLI), USRIN, VOL, VPRO, VTIM, WENG, WPRO, XEST, XMLI, XMLS, XSDF, XSEK

### 9.2.3. Partially Stirred Reactor

The following keywords can be used to build an input file for a PaSR Reactor Model:

ADAM, ATOL, BDF, CFL, CHEM, CMIX, CPROD, CURL, DASP, DT, DT0, DTMX (transient), DTSV, END, EQUI, FLRT, IEM, INIT, INLET, KOUT, MAXIT, MAXTIME, MIX, MIXT, NCFIT, NDPR, NEWRUN, NNEG, NOJC, NPAR, NPIN, PDF, PRES, REAC, RLGAS, RLMIX, RELAXC, RSTR, RTOL, SCAT, SIZE, SSMAXITER, TAU, TEMP, TIME, TINL, TRES, TRMAXITER, VOL, VPRO, WELL, XMLI, XMLS

## 9.3. Flow Reactor Models

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### 9.3.1. Plug Flow Reactor

The following keywords can be used to build an input file for a PFR Reactor Model:

ABFR, ACHG, ADAP, ADD, ADIA, AFLO, AFRA, AINT, AREA, AREAF, AREAQ, AROP, ASEN, ASTEPS, ATLM, ATLS, ATOL, AVALUE, AVAR, BETA, BLKEQ, BULK, CLSC, CLSM, CNTN, CNTX, COLR, CPROD, DIST, DPRO, DTIGN, DX, DXMX, DXSV, EGRR, END, ENRG, EPSG, EPSR, EPSS, EPST, EQUI, ETCH, FLRT, FPRO, FUEL, GFAC, GMHTC, HTC, HTRN, IPSR, KLIM, MCUT, MMASS, MOMEN, NADAP, NEWRUN, NMOM, NNEG, NOCG, NSOL, OXID, PBDEN, PLUG, PNDE, PNDI, PPRO, PRES, PRNT, PROE, PROI, PSV, PTM\_SECTION\_NUM, PTM\_SECTION\_SIZEDEP\_A0, PTM\_SECTION\_SIZEDEP\_COLEFF, PTM\_SECTION\_SIZEDEP\_DSTAR, PTM\_SECTION\_SIZEDEP\_HAMAKER, PTM\_SECTION\_SN0, PTM\_SECTION\_SPACING, PTM\_SECTION\_TCOND, PTM\_SECTION\_USERBULKROP, PTM\_SECTIONAL, PVFE, PVFI, QFUN, QLOS, QPRO, QRGEQ, QRSEQ, RCHG, REAC, RLGAS, RLMIX, ROP, RSTR, RTIME, RTLM, RTLS, RTOL, SCCMPRO, SCLM, SCLS, SCOR, SENG, SFAC, SIZE, SSKIP, SSTT, SURF, TAMB, TEMP, TGIV, TIFP, TLIM, TPRO, TRST, TSRF, TSTP, TSTR, UIGN, USET, USEV (Restart), USEV (XMLI), VDOT, VDOTPRO, VEL, VIS, WENG, XEND, XMLI, XMLS, XRES, XSTR

### 9.3.2. Plasma Plug Flow Reactor

The following keywords can be used to build an input file for a Plasma PFR Reactor Model:

ACHG, ADAP, ADIA, AFLO, AFRA, AINT, AREA, AREAF, AREAQ, AROP, ASEN, ASTEPS, ATLS, AVALUE, AVAR, BETA, BLKEQ, BOHM, BPWR, BULK, CLSC, CLSM, CNTN, CNTX, COLR, CPROD, DIAM, DIST, DPRO, DTIGN, DX, DXMX, DXSV, EGRR, ELSH, END, ENGE, ENRG, EPSG, EPSR, EPSS, EPST, EQUI, ETCH, ETMP, FLRT, FPRO, FUEL, GFAC, GMHTC, HTC, HTRN, IONE, IPSR, KLIM, MAXIT, MCUT, MMASS, MOMEN, NADAP, NEWRUN, NMOM, NNEG, NOCG, NSOL, OXID, PLUG, PNDE, PNDI, PPRO, PRES, PRNT, PROD, PROE, PROI, PSURF, PSV, PVFE, PVFI, PWRW, QFUN, QLOS, QLSE, QPRO, QRGEQ, QRSEQ, RCHG, REAC, RELAXC, ROP, RSTR, RTIME, RTLS, SCCMPRO, SCLM, SCLS, SCOR, SENG, SENT, SFAC, SIZE, SOLUTION\_TECHNIQUE, SSKIP, SURF, TAMB, TEBND, TEMP, TGIV, TIFP, TION, TLIM, TPRO, TRST, TSRF, TSTP, TSTR, UIGN, USET, USEV (Restart), USEV (XMLI), VDOT, VDOTPRO, VELPRO, VIS, WENG, WPRO, XEND, XMLI, XMLS, XRES, XSDF, XSEK, XSTR

### 9.3.3. Planar Shear Flow

The following keywords can be used to build an input file for a Planar Shear Flow Reactor Model:

ABFR, AFLW, AFRA, ADIA, ATIM, ATLM, ATOL, BETA, BULK, CLSC, CLSM, CNTN, COLR, CPROD, DTMN, DTMX (steady-state), DX, DXMX, DXSV, END, FIXT, GASW, GFAC, GRAV, H0, HITE, HTRN, ICRD, IPSR, IRET, ISTP, KNMN, MAXIT, MAXTIME, MCUT, MIX, MORD, MULT, NEWRUN, NJAC, NMOM, NOCG, NOTP, NPTS, NSOL, PARP, PNDE, PNDI, PRES, PRNT, PROE, PROI, PVFE, PVFI, QLOS, QPRO, REAC, RLGAS, RLMIX, RELAXC, RSTR, RTIM, RTLM, RTOL, SFAC, SIZE, SLIP, SQRX, SSMAXITER, SSRX, STCH, STP0, SURF, SYMT, TDIF, TINF, TINL, TJAC, TPRO, TRMAXITER, TSPL, TSRF, TSTR, TWAB, TWPR, TWRE, TWST, UPROF, USET, USEV, UTRN, VCOR, VEL, VWALL, XEND, XMLI, XMLS, XRST, XTMP

### 9.3.4. Cylindrical Shear Flow

The following keywords can be used to build an input file for a Cylindrical Shear Flow Reactor Model:

ABFR, ADIA, AFRA, ATIM, ATLM, ATOL, BETA, BULK, CLSC, CLSM, COLR, CNTN, CPROD, DIST, DTMN, DTMX (steady-state), DX, DXMX, DXSV, END, GASW, GFAC, GRAV, H0, HITE, HTRN, ICRD, IPSR, IRET, ISTD, KNMN, MAXIT, MAXTIME, MCUT, MIX, MORD, MULT, NEWRUN, NJAC, NMOM, NOCG, NOTP, NPTS, NSOL, PARP, PNDE, PNDI, PRES, PRNT, PROE, PROI, PVFE, PVFI, QLOS, QPRO, REAC, RL GAS, RLMIX, RELAXC, RSTR, RTIM, RTLM, RTOL, SFAC, SIZE, SLIP, SQRX, SS MAXITER, SSRX, STCH, STPO, SURF, TDIF, TINF, TINL, TJAC, TPRO, TR MAXITER, TSPL, TSRF, TSTR, TWAB, TWPR, TWRE, TWST, UPROF, USET, USEV, UTRN, VCOR, VEL, VWALL, XEND, XMLI, XMLS, XRST, XTMP

### 9.3.5. Honeycomb Monolith Reactor

The Honeycomb Monolith Reactor Model is a special case of a general plug-flow reactor, where user input parameters describing the honeycomb geometry are used to automatically calculate the available surface area for gas-surface reactions. For details on the calculations performed for the Honeycomb Monolith Reactor Model, see [Honeycomb Monolith Reactor Calculations](#) of the [Chemkin-Pro Theory Manual](#).

The following keywords can be used to build an input file for a Honeycomb Monolith Reactor Model:

ACHG, ADAP, ADIA, AEXT, AFLO, AFRA, AINT, AREA, AREAF, AREAQ, AROP, ASEN, ASTEPS, ATLS, ATOL, AVALUE, AVAR, BETA, BLKEQ, BULK, CLSC, CLSM, CNTN, CNTX, COLR, CPROD, DIAM, DIST, DPRO, DTIGN, DX, DXMX, DXSV, EGRR, END, ENRG, EPSG, EPSR, EPSS, EPST, EQUI, ETCH, FLRT, FPRO, FUEL, GFAC, GMHTC, HTC, HTRN, IPSR, KLIM, MAXIT, MCUT, MMAS, MOMEN, NADAP, NMOM, NNEG, NOCG, NSOL, OXID, PLUG, PNDE, PNDI, PPRO, PRES, PRNT, PROE, PROI, PSURF, PSV, PVFE, PVFI, QFUN, QLOS, QPRO, QRGEQ, QRSEQ, RCHG, REAC, RL GAS, RLMIX, RELAXC, ROP, RSTR, RTIM, RTIME, RTLS, RTOL, SCCM PRO, SCLM, SCLS, SCOR, SENG, SENT, SFAC, SIZE, SOLUTION\_TECHNIQUE, SSKIP, SSTT, SURF, TAMB, TEMP, TGIV, TIFP, TLIM, TPRO, TRST, TSRF, TSTP, TSTR, UIGN, USET, USEV (Restart), USEV (XMLI), VDOT, VDOTPRO, VEL, VIS, WENG, XEND, XMLI, XMLS, XRES, XSTR

## 9.4. Flame Simulators

### 9.4.1. Premixed Laminar Burner-stabilized Flame Simulator

The following keywords can be used to build an input file for a Premixed Laminar Burner-stabilized Flame Simulator:

AGGA, AGGB, AGGD, AGGE, AGGFD, AGGMN, APRO, ASEN, ATIM, ATOL, BURN, CDIF, CNTN, CPROD, CURV, DFAC, DIST, DTMN, DTMX (steady-state), EMPAR, END, ENRG, EPSS, FLRT, FLTB, FLT\_PVSPEC, FLXB, GFAC, GRAD, GRID, HSEN, INTM, IRET, ISTD, JJRG, KOUT, MAXTIME, MIX, MSFX, MULT, NADP, NJAC, NOAGG, NOFT, NOTP (Reactor), NPTS, NSOL, NTOT, PENG, PFLR, PPRO, PRES, PRMN, PRNT, PROD, PSURF, PTM\_SECTION\_NUM, PTM\_SECTION\_SIZEDEP\_A0, PTM\_SECTION\_SIZEDEP\_COEFF, PTM\_SECTION\_SIZEDEP\_DSTAR, PTM\_SECTION\_SIZEDEP\_HAMAKER, PTM\_SECTION\_SN0, PTM\_SECTION\_SPACING, PTM\_SECTION\_TCOND, PTM\_SECTION\_USERBULKROP, PTM\_SECTIONAL, QFUN, RACTV, RADGS, RADPT, REAC, RL GAS, RLMIX, RSTR, RTIM, RTOL, SCLM, SCLS, SENT, SFLR, SFMN, SG MAXIT, SGTOL, SIZE, SOLUTION\_TECHNIQUE, SPOS, SS MAXITER, TBND, TDIF, TEMP, TGIV, TIM1, TIM2, TINF, TJAC, TPRO, TPROF, TRAN, TRCE, TR MAXITER, TSTR, TUNBURNT, USE\_TPRO\_GRID, USET, USEV (Restart), USEV (XMLI), UTRN, VCOR, WDIF, WMIX, XCEN, XEND, XIMN, XMLI, XMLS, XSTR



### 9.4.2. Flame Speed Simulator

The following keywords can be used to build an input file for a Flame Speed Simulator:

ASEN, ATIM, ATOL, CDIF, CNTN, CPROD, CURV, DFAC, DIST, DTMN, DTMX (steady-state), EMPAR, END, ENRG, EPSS, FLRT, FLTB, FLT\_PVSPEC, FLXB, FREE, GFAC, GRAD, GRID, HSEN, INTM, IPSR, IRET, ISTD, JJRG, KOUT, MAXTIME, MIX, MSFX, MULT, NADP, NJAC, NOAGG, NOFT, NOTP (Reactor), NPTS, NSOL, NTOT, PENG, PFLR, PRES, PRMN, PRNT, PROD, PSURF, PTM\_SECTION\_NUM, PTM\_SECTION\_SIZEDEP\_A0, PTM\_SECTION\_SIZEDEP\_COLEFF, PTM\_SECTION\_SIZEDEP\_DSTAR, PTM\_SECTION\_SIZEDEP\_HAMAKER, PTM\_SECTION\_SN0, PTM\_SECTION\_SPACING, PTM\_SECTION\_TCOND, PTM\_SECTION\_USERBULKROP, PTM\_SECTIONAL, QFUN, RACTV, RADGS, RADPT, REAC, RLGAS, RLMIX, RSTR, RTIM, RTOL, SCLM, SCLS, SENT, SFLR, SFMN, SGMAXIT, SGTOL, SIZE, SOLUTION\_TECHNIQUE, SPOS, SSMAXITER, TDIF, TEMP, TFIX, TIM1, TIM2, TINF, TJAC, TPRO, TPROF, TRAN, TRCE, TRMAXITER, TSTR, TUNBURNT, USET, USE\_TPRO\_GRID, USEV (Restart), USEV (XMLI), UTRN, VCOR, WDIF, WMIX, XCEN, XEND, XIMN, XMLI, XMLS, XSTR

### 9.4.3. Opposed-flow Flame Simulator

The following keywords can be used to build an input file for an Opposed-flow Flame Simulator:

AGGA, AGGB, AGGD, AGGE, AGGFD, AGGMN, AINL, ASEN, ATIM, ATOL, AXIS, CDIF, CNTN, CPROD, CURV, DFAC, DIST, DTMN, DTMX (steady-state), EMPAR, END, ENRG, ENTH\_DELTA\_IN, EPSS, FLTB, GFAC, GRAD, GRID, HSEN, INLET, IPSR, IRET, ISTD, JJRG, KOUT, MAXTIME, MIX, MULT, NADP, NDPR, NJAC, NOAGG, NOFT, NOTP (Reactor), NPTS, NSOL, NTOT, PENG, PFLR, PLAN, PLAT, PPRO, PRES, PRNT, PROD, PSURF, PTM\_SECTION\_NUM, PTM\_SECTION\_SIZEDEP\_A0, PTM\_SECTION\_SIZEDEP\_COLEFF, PTM\_SECTION\_SIZEDEP\_DSTAR, PTM\_SECTION\_SIZEDEP\_HAMAKER, PTM\_SECTION\_SN0, PTM\_SECTION\_SPACING, PTM\_SECTION\_TCOND, PTM\_SECTION\_USERBULKROP, PTM\_SECTIONAL, QFUN, RACTV, RADGS, RADPT, REAC, RLGAS, RLMIX, RSTR, RTIM, RTOL, SENT, SFLR, SFMN, SGMAXIT, SGTOL, SIZE, SOLUTION\_TECHNIQUE, SPOS, SSMAXITER, TDIF, TEMP, TGIV, TIM1, TIM2, TINF, TINL, TJAC, TMAX, TPRO, TRAN, TRMAXITER, TSFR, TSTR, UFAC, UINL, USET, UTRN, WDIF, WMIX, XCEN, XEND, XMLI, XMLS

### 9.4.4. Premixed Laminar Burner-stabilized Stagnation Flow Flame Simulator

The following keywords can be used in addition to those listed in [Opposed-flow Flame Simulator](#) (p. 120), [Opposed-flow Flame Simulator](#) (p. 120), to build an input file for a Premixed Laminar Burner-stabilized Stagnation Flow Flame Simulator:

ENTH\_DELTA\_IN, PTM\_SECTION\_NUM, PTM\_SECTION\_SIZEDEP\_A0, PTM\_SECTION\_SIZEDEP\_COLEFF, PTM\_SECTION\_SIZEDEP\_DSTAR, PTM\_SECTION\_SIZEDEP\_HAMAKER, PTM\_SECTION\_SN0, PTM\_SECTION\_SPACING, PTM\_SECTION\_TCOND, PTM\_SECTION\_USERBULKROP, PTM\_SECTIONAL, RLGAS, RLMIX, SCLM, SCLS, STAGNATION\_FLAME, TINL

### 9.4.5. Flame-Extinction Simulator

The following keywords can be used in addition to those listed in [Opposed-flow Flame Simulator](#) (p. 120), [Opposed-flow Flame Simulator](#) (p. 120), to build an input file for a Flame-Extinction Simulator:

ENTH\_DELTA\_IN, EXTINCTION, EXT\_MAXTFRAC, EXT\_METHOD, EXT\_MINTFLAME, EXT\_MINTFRAC, EXT\_SAVEINT, EXT\_STEPS, EXT\_TSTEP, EXT\_VFCNTRL, RLGAS, RLMIX, SCLM, SCLS



### 9.4.6. Diffusion Flamelet Generator

ATOL, ENDTIMEMAX, ENTH\_DELTA\_IN, FLTB, IGRIDMETHOD\_n, INLET, MIXFRACBIAS\_FUEL, MIXFRACBIAS\_OXID, NP\_FUEL, NP\_OXID, NPTS, NSTEPS\_HIGH, NSTEPS\_LOW, NTOT, PRES, REAC, RTOL, SDDR, SDDR\_MAX, SDDR\_MIN, TIME, TINL, TMAX, TPROFILE\_n

## 9.5. CVD Reactors

### 9.5.1. Stagnation Flow CVD Reactor

The following keywords can be used to build an input file for a Stagnation Flow CVD Reactor Model:

AINL, ASEN, ATIM, ATOL, BULK, CDCT, CHEM, CNDT, CNDX, CNTN, COMP, COND, CPROD, CTOL, CURV, DELT, DFAC, DIST, DT0, DTMN, DTMX (steady-state), EMIS, EMSG, END, ENRG, EPSS, ETCH, FLAM, FLRT, FLUX, FPRO, GDOT, GFAC, GRAD, GRID, HSEN, INIT, INJM, INJS, INJT, INJW, INJX, INLET, INTM, IPSR, IRET, ISTP, JJRG, LINE, LPRT, MAXIT, MAXTIME, MIX, MORD, MULT, NADP, NEWRUN, NJAC, NOCH, NOFT, NONR, NOTP, NPTS, NSOL, NTOT, PRES, PRNT, PROD, PWRC, QDOT, QDTC, RADGS, RDSK, REAC, RELAXC, REOR, RLGAS, RLMIX, RRAD, RSTR, RTIM, RTOL, SCCM, SCCMPRO, SENT, SFAC, SFLR, SIZE, SPOS, SSMAXITER, STAG, STST, SURF, TBND, TDIF, TDSK, TEMP, TGIV, TIM1, TIM2, TIME, TINL, TJAC, TOFF, TPRO, TRAD, TRAN, TRCE, TRMAXITER, TSCCM, TSTR, TWAL, UFAC, UINL, USET, USEV (Restart), USEV (XMLI), UWGT, VCOR, WMIX, WSRC, XCEN, XEND, XMLI, XMLS, XSRC, XSTR

### 9.5.2. Rotating Disk CVD Reactor

The following keywords can be used to build an input file for a Rotating Disk CVD Reactor Model:

AINL, ASEN, ATIM, ATOL, BULK, CDCT, CHEM, CNDT, CNDX, CNTN, COMP, COND, CPROD, CTOL, CURV, DELT, DFAC, DIST, DT0, DTMN, DTMX (steady-state), EMIS, EMSG, END, ENRG, EPSS, ETCH, FLAM, FLRT, FLUX, FPRO, GDOT, GFAC, GRAD, GRID, HSEN, INIT, INJM, INJS, INJT, INJW, INJX, INLET, INTM, IPSR, IRET, ISTP, JJRG, LINE, LPRT, MAXIT, MAXTIME, MIX, MORD, MULT, NADP, NEWRUN, NJAC, NOCH, NOFT, NONR, NOTP, NPTS, NSOL, NTOT, OINL, OMEG, PRES, PRNT, PROD, PWRC, QDOT, QDTC, RADGS, RDSK, REAC, RELAXC, REOR, RLGAS, RLMIX, RRAD, RSTR, RTIM, RTOL, SCCM, SCCMPRO, SENT, SFAC, SFLR, SIZE, SPOS, SSMAXITER, STST, SURF, TBND, TDIF, TDSK, TEMP, TGIV, TIM1, TIM2, TIME, TINL, TJAC, TOFF, TPRO, TRAD, TRAN, TRCE, TRMAXITER, TSCCM, TSTR, TWAL, UFAC, UINL, USET, USEV (Restart), USEV (XMLI), UWGT, VCOR, WMIX, WSRC, XCEN, XEND, XMLI, XMLS, XSRC, XSTR

## 9.6. Shock Tube Reactors

### 9.6.1. Normal Incident Shock

The following keywords can be used to build an input file for a Incident Shock Reactor Model:

ATOL, CNTN, CONC, DELT, DIA, DIST, END, INIT, IPSR, ISHK, ISKB, LGDT, NEWRUN, NSOL, P1A, P2A, RHO1, RHO2, RLGAS, RLMIX, RTOL, SIZE, T1, T2, TIME, TSTR, TSTR, USET, VISC, VSHK, XMLI

### 9.6.2. Normal Reflected Shock

The following keywords can be used to build an input file for a Reflected Shock Reactor Model:

ATOL, CNTN, CONC, DELT, DIST, END, INIT, IPSR, LGDT, NEWRUN, NSOL, P1A, P2A, P3A, RHO1, RHO2, RHO3, RLGAS, RLMIX, RSHK, RTOL, SIZE, T1, T2, T3, TIME, TSTR, TSTR, USET, VRS, VSHK, XMLI

## 9.7. Miscellaneous Reactor Models

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### 9.7.1. Gas Mixer

The following keywords can be used to build an input file for a Gas Mixer Reactor Model:

ABSL, ATIM, ATOL, CNTN, CNTT, CPROD, DELT, DFAC, DIST, DTMN, DTMX (steady-state), DTSV, END, ENRG, FLRT, FPRO, GFAC, GMHTC, HTC, HTRN, INLET, IPSR, IRET, ISTP, MAXTIME, MMASS, NEWRUN, NJAC, NNEG, NOFT, NPSR, NSOL, PPRO, PRES, PRNT, QFUN, QLOS, REAC, RELT, RTIM, RTOL, SCCM, SCCMPRO, SCOR, SFAC, SFLR, SIZE, SPOS, SSMAXITER, STPT, STST, TAMB, TEMP, TGIV, TIM1, TIM2, TIME, TINL, TJAC, TPRO, TRAN, TRMAXITER, TSCCM, TSTR, TTIM, UFAC, USET, USEV, USRIN, VOL, VPRO, VTIM, WENG, XMLI, XMLS

### 9.7.2. Equilibrium

The following keywords can be used to build an input file for a Equilibrium Reactor Model:

CJ, CONX, CPROD, DIST, END, ENGY, ENTH, ENTR, FAZE, FREE, FROZ, IPSR, NEWRUN, NSOL, PEST, PH, PRES, PS, PV, REAC, RLGAS, RLMIX, SIZE, TEMP, TEST, TP, TS, TSTR, TV, USET, VH, VOL, VS, VU, XMLI

### 9.7.3. Mechanism Analyzer

The following keywords can be used to build an input file for a Mechanism Analyzer:

ALL, CARR, DIST, END, GEN, GRXN, GTHB, IPSR, LSCL, MAJ, NEWRUN, NONE, NSOL, PFAL, PHIA, PLOA, PNUM, PRES, SCOV, SIZE, SRXN, STCK, TBTH, TBTH, TDEL, TFAL, THIG, THRM, TLOW, TRAN, TSTR, TSUM, USET, XBTH, XMLI

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## Chapter 10: Alphabetical Listing of Project Input Keywords

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In this chapter we provide detailed information about the meaning and usage of each keyword entry that may be included as part of a Reactor Model input file. [Reference Guide to Project Input Keywords](#) (p. 115) provides a cross-referenced listing that shows which keywords are available for each Reactor Model, while [CHEMKIN Project Input: Keyword Syntax and Rules](#) (p. 113) provides general keyword syntax and rules. The following categorized lists of auxiliary keywords are provided:

- [Table 3.4: Alphabetical Listing of REACTIONS-line Options for Gas-phase Kinetics Data](#) (p. 39)
- [Table 3.7: Alphabetical Listing of Gas-phase Reaction Auxiliary Keywords](#) (p. 43)
- [Table 4.3: Alphabetical Listing of REACTIONS-line Options for Surface Reaction Data](#) (p. 66)
- [Table 4.6: Alphabetical Listing of Surface Reaction Auxiliary Keywords](#) (p. 72)

The alphabetical listing of keywords is distributed over the following sections:

[10.1. Alphabetical Listing of Keywords \[A-E\]](#)

[10.2. Alphabetical Listing of Keywords \[F-O\]](#)

[10.3. Alphabetical Listing of Keywords \[P-S\]](#)

[10.4. Alphabetical Listing of Keywords \[T-Z\]](#)

### 10.1. Alphabetical Listing of Keywords [A-E]

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**Table 10.1: Alphabetical Listing of Keywords [A-E]**

Keyword	Definition			
AB- FR  Solver	This keyword serves as a switch to turn on an empirical active surface area factor when surface reaction rates on the particle surface are calculated. The concept is that not all surface area (or sites) on the particle surface is active. The active surface area during the particle formation phase is found to be a function of total particle mass and gas temperature. The form and the model parameters of this empirical formulation are obtained by fitting predictions to measured data from premixed flames. By default this factor is turned off.			
	Parameters	Optional/Reqd.	Units	Examples
	--	--	--	ABFR
	<b>Keyword Usage</b>	Optional keyword. By default this factor is turned off.		
	<b>Reactor Models</b>	<ul style="list-style-type: none"><li>• Cylindrical Shear Flow Reactor</li><li>• Planar Shear Flow Reactor</li><li>• Perfectly-stirred Reactor (PSR)</li><li>• Plug-flow Reactor (PFR)</li></ul>		

Keyword	Definition			
ABSL Solver	This keyword is used to override the default value for the absolute perturbation in the solution variable used in the determination of the numerically derived Jacobian.			
	Parameters	Optional/Reqd.	Units	Examples
	Absolute perturbation	Required	--	ABSL <b>1.E-15</b>
	Keyword Usage	Optional keyword. By default, if the <b>ATOL</b> keyword is given, then the absolute perpetuation is set equal to the <b>ATOL</b> value. <b>ATOL</b> is not specified, then the absolute perturbation is set equal to the square root of the unit round-off error of the machine.		
	Reactor Models	<ul style="list-style-type: none"><li>• Closed Plasma Reactor</li><li>• Non-reactive Gas Mixer</li><li>• Perfectly Stirred Reactor (PSR)</li><li>• Plasma PSR</li></ul>		
ACHG Solver	Maximum absolute change in the surface site fractions (over one time step) for which the preliminary, fictitious transient equations can be considered to have converged to steady state. The convergence test is made against the sum of the <b>ACHG</b> value plus the product of <b>RCHG</b> multiplied by the old site-fraction value. Therefore, if <b>ACHG</b> is set to zero (by default) then only <b>RCHG</b> is used to control the convergence criteria.			
	Parameters	Optional/Reqd.	Units	Examples
	Absolute relative change	Required	--	ACHG <b>1.0E-7</b>
	Keyword Usage	Optional keyword. By default, only <b>RCHG</b> is used to determine convergence.		
	Reactor Models	<ul style="list-style-type: none"><li>• Honeycomb Reactor</li><li>• Plasma Plug Flow Reactor</li><li>• Plug Flow Reactor</li></ul>		
ADAM Solver	Flag indicating the implicit Adams method of the DVODE solver is used to integrate the equations.			
	Keyword Usage	Optional keyword. By default, the DASPK solver will be used.		
	Reactor Models	<ul style="list-style-type: none"><li>• Closed Partially Stirred Reactor (PaSR)</li><li>• Partially Stirred Reactor (PaSR)</li></ul>		
ADAP Solver	Flag indicating the saving of additional adaptive points for improved resolution of the solution data (e.g., for post-processing and plotting) for transient simulations. ADAP is the default. ADAP inserts extra solution points when your solution is changing rapidly (e.g., a steep transient or engine ignition occurs).			

Keyword	Definition			
	How and when the points are inserted is controlled by the <a href="#">AVALUE</a> , <a href="#">AVAR</a> and <a href="#">ASTEPS</a> keywords. The companion keyword, <a href="#">NADAP</a> , can be used to turn off adaptive time-stepping during continuations, if desired.			
	Keyword Usage	Optional keyword. ADAP is the default.		
	Reactor Models	<ul style="list-style-type: none"><li>• Closed Plasma Reactor</li><li>• Closed Homogeneous Reactor</li><li>• Honeycomb Reactor</li><li>• IC HCCI Engine Model</li><li>• Multi-Zone HCCI Engine Simulator</li><li>• Plasma Plug Flow Reactor</li><li>• Plug Flow Reactor</li><li>• SI Engine Zonal Simulator</li></ul>		
ADD  Reactor or Inlet Property	Mole fractions of species that should be added to the inlet or initial composition but excluded from the equivalence-ratio calculation. This keyword is only valid when the equivalence-ratio option is used to specify the inlet or initial composition. These species do not enter into the equivalence ratio computations. One species is entered per line.			
	Parameters	Optional/Reqd.	Units	Examples
	Inlet stream name	Optional (PSRs only) If there is no stream name than the product species applies to the default or all defined streams.	--	ADD <b>mixture1</b> AR 0.2
	Species name	Required	--	ADD <b>AR</b> 0.2
	Additive fractions	Required	mole fractions	ADD AR <b>0.2</b>
	Keyword Usage	Optional keyword. By default, <a href="#">ADD</a> is not used. But either <a href="#">REAC</a> or <a href="#">EQUI</a> / <a href="#">FUEL</a> / <a href="#">OXID</a> / <a href="#">CPROD</a> is required for each inlet stream or to define initial conditions for a closed system.		

Keyword	Definition			
	<b>Reactor Models</b>	<ul style="list-style-type: none"><li>• Closed Homogeneous Batch Reactor</li><li>• IC HCCI Engine</li><li>• Plasma PSR</li><li>• Plug Flow Reactor</li><li>• SI Engine Zonal Simulator</li></ul>		
	<b>Notes</b>	<ul style="list-style-type: none"><li>• The <a href="#">ADD</a> keywords must be changed as a set, not individually for a restart run.</li><li>• The <a href="#">ADD</a> keywords must be changed as a set, not individually for a continuation run.</li></ul>		
<b>ADIA</b>  Reactor Property	Turns on the adiabatic wall condition for plug-flow or for planar, symmetric, shear-flow models. For planar, non-symmetric shear flow, an adiabatic wall is the default, but for symmetric (planar or cylindrical) shear-flow cases, the <a href="#">ADIA</a> keyword is required for the adiabatic condition.			
	<b>Keyword Usage</b>	Optional keyword. By default, the specified (temperature) condition is used for shear-layer flow. The default behavior for plug-flow depends on the problem type; if the energy equation is being solved, the default is for adiabatic conditions.		
	<b>Reactor Models</b>	<ul style="list-style-type: none"><li>• Cylindrical Shear Flow Reactor</li><li>• Honeycomb Reactor</li><li>• Planar Shear Flow Reactor</li><li>• Plasma Plug Flow Reactor</li><li>• Plug Flow Reactor</li></ul>		
<b>AEXT</b>  Reactor Property Profiles	External surface area (for 0-D Homogeneous systems) or surface area per unit length (for Plug Flow Models) used to control heat transfer to the external environment. <a href="#">AEXT</a> is usually used to specify area profiles as a function of time (0-D Homogeneous systems) or distance (Plug Flow Models). However, if the <a href="#">AEXT</a> value is only provided at a single point, then the surface area is assumed to be constant as a function of time (for transient 0-D Homogeneous systems) or distance (for Plug Flow Models). See also <a href="#">AREAQ</a> .			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Time or Distance, depending on Reactor Model</i>	Required	sec or cm	AEXT <b>0.0</b> 1.0
	<i>External surface area or surface area per unit length,</i>	Required	cm <sup>2</sup> or cm	AEXT 0.0 <b>1.0</b>

Keyword	Definition			
	<i>depending on Reactor Model</i>			
	Keyword Usage	Optional keyword. If not specified, the external area is assumed equal to the internal surface area (see <a href="#">AINT</a> or <a href="#">AREA</a> ).		
	Reactor Models	<ul style="list-style-type: none"><li>• Closed Homogeneous Batch Reactor</li><li>• Closed Plasma Reactor</li><li>• Honeycomb Reactor</li><li>• IC HCCI Engine</li><li>• Perfectly Stirred Reactor (PSR)</li><li>• Plasma PSR</li><li>• SI Engine Zonal Simulator</li></ul>		
AFLO  Reactor Property Profiles	Cross-sectional area profile as a function of distance. If only a single <a href="#">AFLO</a> entry is provided, the cross-sectional area is assumed to be a constant at that specified value. See also <a href="#">AREAF</a> and <a href="#">DIAM</a> .			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Distance from inlet</i>	Required	cm	AFLO <b>0.0</b> 1.0
	<i>Cross-sectional area</i>	Required	cm <sup>2</sup>	AFLO 0.0 <b>1.0</b>
	Keyword Usage	Optional keyword. If none of <a href="#">DIAM</a> , <a href="#">AFLO</a> , or <a href="#">AREAF</a> keywords are included, then an attempt will be made to use the GEOM user subroutine to determine the flow area.		
	Reactor Models	<ul style="list-style-type: none"><li>• Honeycomb Reactor</li><li>• Plasma Plug Flow Reactor</li><li>• Plug Flow Reactor</li></ul>		
AFLW  Reactor Property	Fraction of the total lower wall surface area that corresponds to a surface material. For example, "AFLW WAFER 0.001" indicates that the material "WAFER" makes up 0.1% of the lower wall surface area. The material name must correspond to a material name declared in the <i>Surface Kinetics</i> input file or an error will occur.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Surface material name</i>	Required	--	AFLW <b>WAFER</b> 0.001
	<i>Fraction of total surface area</i>	Required	--	AFLW WAFER <b>0.001</b>
	Keyword Usage	Optional keyword. By default, 1.0 is used for all materials in all PSRs.		
	Reactor Models	<ul style="list-style-type: none"><li>• Non-symmetric Planar Shear Flow Reactor</li></ul>		

Keyword	Definition			
AFRA  Reactor Property	Fraction of the total surface area that corresponds to a surface material (see the multiple surface material capability under <i>Surface Kinetics</i> ). For example, “AFRA WAFER 0.001” indicates that the material “WAFER” makes up 0.1% of the total reactor surface area. The material name must correspond to a material name declared in the <i>Surface Kinetics</i> input file or an error will occur.			
	Parameters	Optional/Reqd.	Units	Examples
	Surface material name	Optional	--	AFRA <b>WAFER</b> 0.001
	Fraction of total surface area	Required	--	AFRA WAFER <b>0.001</b>
	Reactor number (PSR clusters only)	Optional  If no number is given, the keyword is assumed to apply to all reactors in a cluster.	--	AFRA WAFER 0.001 <b>2</b>
	Keyword Usage	Optional keyword. By default, 1.0 is used for all materials in all PSRs.		
	Reactor Models	<ul style="list-style-type: none"><li>• Closed Homogeneous Batch Reactor</li><li>• Closed Plasma Reactor</li><li>• Cylindrical Shear Flow Reactor</li><li>• Honeycomb Reactor</li><li>• Perfectly Stirred Reactor (PSR)</li><li>• Planar Shear Flow Reactor</li><li>• Plasma Plug Flow Reactor</li><li>• Plasma PSR</li><li>• Plug Flow Reactor</li></ul>		
AFRMX  Reactor Property/Model	Maximum air entrainment mass flow rate into the spray parcel.			
	Parameters	Optional/Reqd.	Units	Examples
	Max air entrainment rate	Required	g/sec	AFRMX <b>200.0</b>
	Keyword Usage	Optional keyword. Default is 50 g/sec.		



Keyword	Definition			
	Reactor Models	• Direct Injection Diesel Engine Simulator		
AGGA  Reactor Property	The pre-exponential factor of the Arrhenius-like expression for characteristic fusion time.			
	Parameters	Optional/Reqd.	Units	Examples
	Material name	Required	--	AGGA <b>SOOT 1.0E10</b>
	Pre-exponential factor	Required	sec	AGGA <b>C(B) 1.0E7</b>
	Keyword Usage	Optional keyword. By default, the pre-exponential factor is 1.0E-30.		
	Reactor Models	• Closed Homogeneous Batch Reactor  • Closed Plasma Reactor  • Diffusion or Premixed Opposed-flow Flame  • IC HCCI Engine  • Multi-Zone HCCI Engine Simulator  • Perfectly Stirred Reactor (PSR)  • Plasma PSR  • Premixed Laminar Burner-stabilized Flame  • SI Engine Zonal Simulator		
AG-GB  Reactor Property	The temperature exponent of the Arrhenius-like expression for characteristic fusion time.			
	Parameters	Optional/Reqd.	Units	Examples
	Material name	Optional	--	AGGB SOOT 1.0
	Temperature exponent	Required		AGGB <b>C(B) 0.5</b>
	Keyword Usage	Optional keyword. By default, the temperature exponent is 0.		
	Reactor Models	• Closed Homogeneous Batch Reactor  • Closed Plasma Reactor  • Diffusion or Premixed Opposed-flow Flame  • IC HCCI Engine  • Multi-Zone HCCI Engine Simulator  • Perfectly Stirred Reactor (PSR)  • Plasma PSR		

Keyword	Definition			
		<ul style="list-style-type: none"><li>• Premixed Laminar Burner-stabilized Flame</li><li>• SI Engine Zonal Simulator</li></ul>		
AG-GD  Reactor Property	The exponent of the primary particle diameter in the Arrhenius-like expression for characteristic fusion time.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Primary particle name</i>	Optional	--	AGGD C(B) 1.0
	Keyword Usage	Optional keyword. By default, the primary particle diameter is 1.0.		
	Reactor Models	<ul style="list-style-type: none"><li>• Closed Homogeneous Batch Reactor</li><li>• Closed Plasma Reactor</li><li>• Diffusion or Premixed Opposed-flow Flame</li><li>• IC HCCI Engine</li><li>• Multi-Zone HCCI Engine Simulator</li><li>• Perfectly Stirred Reactor (PSR)</li><li>• Plasma PSR</li><li>• Premixed Laminar Burner-stabilized Flame</li><li>• SI Engine Zonal Simulator</li></ul>		
AGGE  Reactor Property	The activation temperature of the Arrhenius-like expression for characteristic fusion time.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Material name</i>	Required	--	AGGE <b>SOOT</b> 0.0
	<i>Activation temperature</i>	Required	K	AGGE C(B) <b>800</b>
	Keyword Usage	Optional keyword. By default, the activation temperature is 0.		
	Reactor Models	<ul style="list-style-type: none"><li>• Closed Homogeneous Batch Reactor</li><li>• Closed Plasma Reactor</li><li>• Diffusion or Premixed Opposed-flow Flame</li><li>• IC HCCI Engine</li><li>• Multi-Zone HCCI Engine Simulator</li><li>• Perfectly Stirred Reactor (PSR)</li><li>• Plasma PSR</li></ul>		

Keyword	Definition			
		<ul style="list-style-type: none"><li>• Premixed Laminar Burner-stabilized Flame</li><li>• SI Engine Zonal Simulator</li></ul>		
AGGFD  Reactor Property	The fractal dimension of the aggregate.			
	Parameters	Optional/Reqd.	Units	Examples
	Material name	Required	--	AGGFD <b>SOOT 1.0E3.0</b>
	Fractal dimension	Required	--	AGGFD <b>C(B) 1.8</b>
	Keyword Usage	Optional keyword. By default, the fractal dimension is 3.0.		
	Reactor Models	<ul style="list-style-type: none"><li>• Closed Homogeneous Batch Reactor</li><li>• Closed Plasma Reactor</li><li>• Diffusion or Premixed Opposed-flow Flame</li><li>• IC HCCI Engine</li><li>• Multi-Zone HCCI Engine Simulator</li><li>• Perfectly Stirred Reactor (PSR)</li><li>• Plasma PSR</li><li>• Premixed Laminar Burner-stabilized Flame</li><li>• SI Engine Zonal Simulator</li></ul>		
AGGMN  Reactor Property	The threshold value to include the sintering effect in particle aggregation. For the Moments Method, this indicates the ratio of the collision to the fusion time scale, whereas for the Sectional Method, this indicates the minimum value of the characteristic fusion time.			
	Parameters	Optional/Reqd.	Units	Examples
	Material name	Required	--	AGGMN <b>SOOT 1.0E10</b>
	Threshold	Required	-- (Moments)sec (Sectional)	AGGMN <b>SOOT 1.0E-4</b>
	Keyword Usage	Optional keyword. By default, the threshold is 1.0E-3 for the Moments Method and 1.0E-06 for the Sectional Method.		
	Reactor Models	<ul style="list-style-type: none"><li>• Closed Homogeneous Batch Reactor</li><li>• Closed Plasma Reactor</li><li>• Diffusion or Premixed Opposed-flow Flame</li><li>• IC HCCI Engine</li><li>• Multi-Zone HCCI Engine Simulator</li></ul>		

Keyword	Definition			
		<ul style="list-style-type: none"><li>• Perfectly Stirred Reactor (PSR)</li><li>• Plasma PSR</li><li>• Premixed Laminar Burner-stabilized Flame</li><li>• SI Engine Zonal Simulator</li></ul>		
AINL  Inlet Property	The radial velocity spreading rate. At the inlet $x = L$ , $v/r = \text{AINL}$ .			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Radial velocity divided by radius</i>	Required	1/sec	AINL <b>2.3</b>
	<b>Keyword Usage</b>	Optional keyword. By default, the radial velocity spreading rate is 0.0.		
	<b>Reactor Models</b>	<ul style="list-style-type: none"><li>• Diffusion or Premixed Opposed-flow Flame</li><li>• Rotating Disk CVD Reactor</li><li>• Stagnation Flow CVD Reactor</li></ul>		
	<b>Notes</b>	<ul style="list-style-type: none"><li>• Supersedes previous <b>AFUE</b> and <b>AOXI</b> keywords.</li></ul>		
AINT  Reactor Property Profiles	Internal surface area (for 0-D Homogeneous systems) or surface area per unit length (for Plug Flow models) that is considered active for surface chemistry. <b>AINT</b> is usually used to specify area profiles as a function of time (0-D Homogeneous systems) or distance (Plug Flow models). However, if the <b>AINT</b> value is only provided at a single point, then the surface area is assumed to be constant as a function of time (for transient 0-D Homogeneous systems) or distance (for Plug Flow models). See also <b>AREA</b> .			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Time or distance, depending on Reactor Model</i>	Required	sec or cm	AINT <b>0.0</b> 1.0
	<i>Internal surface area or area per unit length, depending on Reactor Model</i>	Required	cm <sup>2</sup> or cm	AINT 0.0 <b>1.0</b>
	<b>Keyword Usage</b>	Optional keyword. If not specified, the internal surface area is determined based on the hydraulic diameter for a plug-flow, as specified through <b>AFLO</b> , <b>AREAF</b> , or <b>DIAM</b> keywords. For 0-D Homogenous systems, a value of 0.0 is assumed by default.		
	<b>Reactor Models</b>	<ul style="list-style-type: none"><li>• Closed Homogeneous Batch Reactor</li><li>• Closed Plasma Reactor</li><li>• Honeycomb Reactor</li></ul>		

Keyword	Definition			
		<ul style="list-style-type: none"><li>• Perfectly Stirred Reactor (PSR)</li><li>• Plasma PSR</li><li>• Plasma Plug Flow Reactor</li><li>• Plug Flow Reactor</li></ul>		
ALL  Output	Turns default output on for all of Surftherm's tables.			
	Keyword Usage	Optional keyword. By default, the all output will be printed. See also <a href="#">NONE</a> .		
	Reactor Models	<ul style="list-style-type: none"><li>• Mechanism Analyzer</li></ul>		
APRO  Reactor Property Profiles	Use of the <a href="#">APRO</a> keyword(s) allow the user to specify a piece-wise linear profile as a function of distance for the stream-tube area. The stream-tube area is given relative to the burner area and is therefore dimensionless. Each input provides a pair and the x coordinates must be in ascending order. For example, APRO 0.1 1.2 assigns a relative area of 1.2 at a position 0.1 cm from the burner surface.			
	Parameters	Optional/Reqd.	Units	Examples
	x-coordinates	Required	cm	APRO <b>0.1</b> 1.2
	Relative area	Required	dimensionless	APRO 0.1 <b>1.2</b>
	Keyword Usage	Optional keyword. By default, the area ratio is constant at 1.0.		
	Reactor Models	<ul style="list-style-type: none"><li>• Premixed Laminar Burner-stabilized Flame</li></ul>		
	Notes	<ul style="list-style-type: none"><li>• This keyword can be changed for a restart run.</li></ul>		
AREA  Reactor Property	The total internal surface area (for 0-D homogeneous reactors) or surface area per unit length (for plug-flow) in the reactor. The internal surface area represents the area available for surface chemistry. See also <a href="#">AINT</a> .			
	Parameters	Optional/Reqd.	Units	Examples
	Total surface area or surface area per unit length, depending on Reactor Model	Required	cm <sup>2</sup> or cm	AREA <b>200</b>
	Reactor number (PSR clusters only)	Optional  If no number is given, the keyword is assumed to apply to all reactors	--	AREA 200 <b>1</b>

Keyword	Definition			
		in a cluster.		
	Keyword Usage	Optional keyword. By default, the total surface area is set to 0.0 for 0-D homogeneous reactor models and is determined based on the hydraulic diameter (set using <a href="#">DIAM</a> , <a href="#">AREAF</a> , <a href="#">AFLO</a> ) for plug-flow.		
	Reactor Models	<ul style="list-style-type: none"><li>• Closed Homogeneous Batch Reactor</li><li>• Closed Plasma Reactor</li><li>• Honeycomb Reactor</li><li>• Perfectly Stirred Reactor (PSR)</li><li>• Plasma PSR</li><li>• Plasma Plug Flow Reactor</li><li>• Plug Flow Reactor</li></ul>		
AREAF	The total cross-sectional flow area. See also <a href="#">AFLO</a> .			
Reactor Property	Parameters	Optional/Reqd.	Units	Examples
	Cross-sectional flow area	Required	cm <sup>2</sup>	AREAF <b>200</b>
	Keyword Usage	Optional keyword. Either <a href="#">DIAM</a> or <a href="#">AREAF</a> must be set, unless the user has implemented the GEOM user subroutine.		
	Reactor Models	<ul style="list-style-type: none"><li>• Honeycomb Reactor</li><li>• Plasma Plug Flow Reactor</li><li>• Plug Flow Reactor</li></ul>		
AREAQ	The total external surface area (for 0-D homogeneous reactors) or surface area per unit length (for plug-flow) in the reactor. The external surface area represents the area available for heat transfer to the external environment. See also <a href="#">AEXT</a> .			
Reactor Property	Parameters	Optional/Reqd.	Units	Examples
	Total surface area or surface area per unit length, depending on Reactor Model	Required	cm <sup>2</sup> or cm	AREAQ <b>200</b>
	Reactor number (PSR clusters only)	Optional  If no number is given, the keyword	--	AREAQ 200 <b>1</b>

Keyword	Definition			
		is assumed to apply to all reactors in a cluster.		
	Keyword Usage	Optional keyword. By default, the total external surface area is set equal to the internal surface area ( <a href="#">AREA</a> , <a href="#">AINT</a> ), unless <a href="#">AREAQ</a> or <a href="#">AEXT</a> are included.		
	Reactor Models	<ul style="list-style-type: none"><li>• Closed Homogeneous Batch Reactor</li><li>• Closed Plasma Reactor</li><li>• Honeycomb Reactor</li><li>• Perfectly Stirred Reactor (PSR)</li><li>• Plasma PSR</li><li>• Plasma Plug Flow Reactor</li><li>• Plug Flow Reactor</li></ul>		
AROP Output	Determine the rate-of-production coefficients for all species and print results to the diagnostic output file of the reactor simulation.			
	Keyword Usage	Optional keyword. By default, no rate-of-production values are printed.		
	Reactor Models	<ul style="list-style-type: none"><li>• Closed Homogeneous Batch Reactor</li><li>• Closed Plasma Reactor</li><li>• Honeycomb Reactor</li><li>• IC HCCI Engine</li><li>• Perfectly Stirred Reactor (PSR)</li><li>• Plasma Plug Flow Reactor</li><li>• Plasma PSR</li><li>• Plug Flow Reactor</li><li>• SI Engine Zonal Simulator</li></ul>		
	Notes	<ul style="list-style-type: none"><li>• This keyword can be added but not removed from a continuation run.</li></ul>		
ASEN	Calculate the first-order, A-factor sensitivity coefficients (i.e., with respect to the gas-phase and surface chemistry rate constants) for species fractions and for			

Keyword	Definition			
Output	other dependent variables in the system. Sensitivity results will be included in the XML Solution File. For 0-D and Plug Flow systems, sensitivity results will also be printed to the diagnostic output file.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>String indicating for which variables sensitivity coefficients will be saved or printed. The string is a space-delimited list containing species names and any one of the following: ALL, AVEL, RVEL, CVEL, FLRT, or TEMP (see Notes)</i>	Optional  If no string is given, then ALL is assumed.	--	ASEN <b>H2O</b>  ASEN <b>TEMP</b>
	<b>Keyword Usage</b>	Optional keyword. By default, no sensitivity coefficients are computed or printed. See also <a href="#">SENG</a> .		
	<b>Reactor Models</b>	<ul style="list-style-type: none"> <li>• Closed Homogeneous Batch Reactor</li> <li>• Closed Plasma Reactor</li> <li>• Diffusion or Premixed Opposed-flow Flame</li> <li>• Honeycomb Reactor</li> <li>• IC HCCI Engine</li> <li>• Perfectly Stirred Reactor (PSR)</li> <li>• Plasma Plug Flow Reactor</li> <li>• Plasma PSR</li> <li>• Plug Flow Reactor</li> <li>• Premixed Laminar Burner-stabilized Flame</li> <li>• Premixed Laminar Flame-speed Calculation</li> <li>• Rotating Disk CVD Reactor</li> <li>• SI Engine Zonal Simulator</li> <li>• Stagnation Flow CVD Reactor</li> </ul>		
	<b>Notes</b>	<ul style="list-style-type: none"> <li>• This keyword can be added but not removed from a continuation run.</li> <li>• See also <a href="#">EPSS</a>, <a href="#">EPSG</a>, <a href="#">EPST</a>, <a href="#">SENG</a>, and <a href="#">HSEN</a> for other sensitivity options</li> </ul>		



Keyword	Definition			
		The optional parameter strings are defined as follows: <ul style="list-style-type: none"><li>• <b>ALL</b>: all species and all other dependent variables in the solution</li><li>• <b>AVEL</b>: axial velocity (Plug Flow, Diffusion or Premixed Opposed-flow Flames, Rotating Disk, and Stagnation Flow CVD Reactors only)</li><li>• <b>CVEL</b>: circumferential velocity (Rotating Disk and Stagnation Flow CVD Reactors only)</li><li>• <b>RVEL</b>: radial velocity (Diffusion or Premixed Opposed-flow Flames, Rotating Disk, and Stagnation Flow CVD Reactors only)</li><li>• <b>FLRT</b>: mass flow rate (Premixed Laminar Flame-speed Calculation only)</li><li>• <b>TEMP</b>: gas temperature</li></ul>		
<b>ASTEPS</b>  Output	Uses the integrator steps to adaptively insert extra solution data points in addition to those specified by the <b>DTSV</b> option whenever the solver takes the number of integration steps specified by this option. The default is 20, the value used if no argument is provided. The purpose of the <b>ASTEPS</b> keyword is to ensure that during a transient solution, sufficient solution data points are available around the time of a fast transient, for example a rapidly increasing temperature, so that an accurate analysis of the problem is possible (to allow a good plotting resolution).			
	Parameters	Optional/Reqd.	Units	Examples
	Integration steps	<b>Optional.</b>	--	<b>ASTEPS 20</b>
	<b>Keyword Usage</b>	Optional keyword. By default <b>ASTEPS</b> is set to 20.		
	<b>Reactor Models</b>	<ul style="list-style-type: none"><li>• Closed Homogeneous Reactor</li><li>• Closed Plasma Reactor</li><li>• Honeycomb Reactor</li><li>• IC HCCI Engine</li><li>• Multi-Zone HCCI Engine Simulator</li><li>• Perfectly Stirred Reactor (PSR)</li><li>• Plasma Plug Flow Reactor</li><li>• Plasma PSR</li><li>• Plug Flow Reactor</li><li>• SI Engine Zonal Simulator</li></ul>		

Keyword	Definition			
	Notes	• For further details, see the description of <a href="#">DTSV</a> .		
AS-WH  Reactor Property	Crank angle at which the simulation switches from fixed-temperature condition to using energy equation with Woschni correlation as the heat transfer model. By default the energy equation is used starting at zero crank angle.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Crank angle in degrees.</i>	Required	degree	ASWH 5.0
	Keyword Usage	Optional keyword.		
	Reactor Models	• Multi-Zone HCCI Engine Simulator  • SI Engine Zonal Simulator		
ATIM  Solver	Absolute tolerance for convergence of Newton iteration as it is used in the pseudo time stepping procedure for steady-state problems employing the <i>Twopnt</i> solver. Since we are not seeking accuracy in a transient solution, this convergence criteria typically does not need to be as stringent as for the Newton iteration on the actual steady-state solution.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Absolute tolerance</i>	Required	--	ATIM <b>1.E-6</b>
	Keyword Usage	Optional keyword. By default, the absolute tolerance is 1.E-9. See also <a href="#">RTIM</a> .		
	Reactor Models	• Closed Plasma Reactor  • Cylindrical Shear Flow Reactor  • Diffusion or Premixed Opposed-flow Flame  • Honeycomb Reactor  • Non-reactive Gas Mixer  • Perfectly Stirred Reactor (PSR)  • Planar Shear Flow Reactor  • Plasma PSR  • Premixed Laminar Burner-stabilized Flame  • Premixed Laminar Flame-speed Calculation  • Rotating Disk CVD Reactor  • Stagnation Flow CVD Reactor		
	Notes	• For a precise definition, see the description of <a href="#">ATOL</a> .		
	ATLM	<a href="#">ATOL</a> is used for all variables.		

Keyword	Definition			
Solver	Parameters	Optional/Reqd.	Units	Examples
	Tolerance	Required	--	ATLM <b>1.0E-6</b>
	Keyword Usage	ATOL.		
	Reactor Models	<ul style="list-style-type: none"><li>• Closed Plasma Reactor</li><li>• Cylindrical Shear Flow Reactor</li><li>• Perfectly Stirred Reactor (PSR)</li><li>• Planar Shear Flow Reactor</li><li>• Plasma PSR</li></ul>		
ATLRE Reactor Property/Model	The absolute tolerance to determine the energy fluxes at the droplet surface are balanced. This is one of the convergence criteria for solving the droplet surface temperature. This parameter is associated with the “Solve for Surface T” option of the vaporization model.			
	Parameters	Optional/Reqd.	Units	Examples
	Tolerance	Required	--	ATLRE <b>1.0E-6</b>
	Keyword Usage	Optional keyword.		
	Reactor Models	<ul style="list-style-type: none"><li>• Direct Injection Diesel Engine Simulator</li></ul>		
ATLS Solver	Absolute tolerance used by the transient DASPK solver, as an indicator of the accuracy desired in the solution for the sensitivity coefficients only. Generally, the sensitivity coefficients need not be solved to a great degree of accuracy, so these tolerances could be lower than the tolerances placed on the physical variables.			
	Parameters	Optional/Reqd.	Units	Examples
	Absolute tolerance	Required	--	ATLS <b>1.E-3</b>
	Keyword Usage	Optional keyword. The default absolute tolerance is 1.E-5.		
	Reactor Models	<ul style="list-style-type: none"><li>• Closed Homogeneous Batch Reactor</li><li>• Closed Plasma Reactor</li><li>• Honeycomb Reactor</li><li>• IC HCCI Engine</li><li>• Perfectly Stirred Reactor (PSR)</li><li>• Plasma PSR</li><li>• Plasma Plug Flow Reactor</li><li>• Plug Flow Reactor</li><li>• SI Engine Zonal Simulator</li></ul>		

Keyword	Definition			
ATLTS  Reactor Property/Model	The absolute tolerance for the droplet surface temperature. A droplet surface temperature is considered found when the change in the droplet surface temperature of two consecutive iterations is less than the tolerance. This parameter is associated with the “Solve for Surface T” option of the vaporization model.			
	Parameters	Optional/Reqd.	Units	Examples
	Temperature change	Required	K	ATLTS <b>0.01</b>
	Keyword Usage	Optional keyword. Default is 0.001 K.		
	Reactor Models	• Direct Injection Diesel Engine Simulator		
ATOL  Solver	Absolute tolerance used by the solvers as an indicator of the accuracy desired in the physical solution. Typically <b>ATOL</b> should be less than the smallest meaningful value of a species mass fraction.			
	Parameters	Optional/Reqd.	Units	Examples
	Absolute tolerance	Required	--	ATOL <b>1.E-9</b>
	Keyword Usage	Optional keyword. The default values are:  CVD, Partially Stirred Reactor (PaSR), Plug Flow Reactor, Shear Flow Reactor: 1.E-8  Open 0-D Reactors run in steady-state mode, Opposed-flow Flame, Premixed Laminar Burner-stabilized Flame, Premixed Laminar Flame-speed Calculation: 1.E-9  Normal Incident Shock, Normal Reflected Shock: 1.E-10  Closed 0-D Reactors and Open 0-D Reactors run in transient mode: 1.E-20  See also <b>RTOL</b> .		
	Reactor Models	• Closed Homogeneous Batch Reactor  • Closed Partially Stirred Reactor (PaSR)  • Closed Plasma Reactor  • Cylindrical Shear Flow Reactor  • Diffusion or Premixed Opposed-flow Flame  • Honeycomb Reactor  • IC HCCI Engine  • Non-reactive Gas Mixer  • Normal Incident Shock		

Keyword	Definition			
		<ul style="list-style-type: none"><li>• Normal Reflected Shock</li><li>• Opposed-flow Flame</li><li>• Partially Stirred Reactor (PaSR)</li><li>• Perfectly Stirred Reactor (PSR)</li><li>• Planar Shear Flow Reactor</li><li>• Plasma PSR</li><li>• Plug Flow Reactor</li><li>• Premixed Laminar Burner-stabilized Flame</li><li>• Premixed Laminar Flame-speed Calculation</li><li>• Rotating Disk CVD Reactor</li><li>• SI Engine Zonal Simulator</li><li>• Stagnation Flow CVD Reactor</li></ul>		
<b>AVALUE</b>  Output	Uses the integrator steps to adaptively insert extra solution data points in addition to those specified by the <b>DTSV</b> option whenever the variable specified by the <b>AVAR</b> keyword moves by $\pm x$ since the last time an extra data point was generated. You must specify a value for AVALUE; there is no default and you must also specify the <b>AVAR</b> keyword. The purpose of the AVALUE keyword is to ensure that during a transient solution, sufficient solution data points are available around the time of a fast transient, for example a rapidly increasing temperature, so that an accurate analysis of the problem is possible (to allow plotting a resolution).			
	Parameters	Optional/Reqd.	Units	Examples
	Integration steps	Required	--	AVALUE 10
	Keyword Usage	Optional keyword. AVAR is required.		
	Reactor Models	<ul style="list-style-type: none"><li>• Closed Plasma Reactor</li><li>• Closed Homogeneous Reactor</li><li>• Honeycomb Reactor</li><li>• IC HCCI Engine Model</li><li>• Multi-Zone HCCI Engine Simulator</li><li>• Perfectly Stirred Reactor (PSR)</li><li>• Plasma Plug Flow Reactor</li><li>• Plasma PSR</li><li>• Plug Flow Reactor</li></ul>		

Keyword	Definition			
		• SI Engine Zonal Simulator		
	Notes	• See also <a href="#">ASTEPS</a> and <a href="#">AVAR</a> is required when AVALUE is used.		
AV-AR  Output	Determines which variable is used for the <a href="#">AVALUE</a> keyword. Parameter <string> should be “temperature” or the name of a particular species to serve as the time-stepping monitor species. There is no default species value. AVAR is required when the <a href="#">AVALUE</a> keyword is used.			
	Parameters	Optional/Reqd.	Units	Examples
	String	Required	--	AVALUE <b>temperature</b>  AVALUE <b>CH4</b>
	Keyword Usage	Optional keyword.		
	Reactor Models	• Closed Plasma Reactor  • Closed Homogeneous Reactor  • Honeycomb Reactor  • IC HCCI Engine Model  • Multi-Zone HCCI Engine Simulator  • Perfectly Stirred Reactor (PSR)  • Plasma Plug Flow Reactor  • Plasma PSR  • Plug Flow Reactor  • SI Engine Zonal Simulator		
AX-IS  Reactor Property	Use a radial, axisymmetric coordinate system.			
	Keyword Usage	Optional keyword. By default, the coordinate system is radially axisymmetric.		
	Reactor Models	• Diffusion or Premixed Opposed-flow Flame		
AZFAC  Reactor Property/Model	The maximum portion of the initial cylinder volume that can be assigned to the spray parcels.			
	Parameters	Optional/Reqd.	Units	Examples
	Maximum total initial parcel volume	Required	--	AZFAC <b>0.33</b>
	Keyword Usage	Optional keyword. Default is 0.5.		
	Reactor Models	• Direct Injection Diesel Engine Simulator		

Keyword	Definition			
BDF Solver	Flag indicating the backward differentiation formulas of the DVODE solver is used to integrate the equations.			
	Keyword Usage	Optional keyword. By default, the DASPK solver will be used.		
	Reactor Models	<ul style="list-style-type: none"><li>Closed Partially Stirred Reactor (PaSR)</li><li>Partially Stirred Reactor (PaSR)</li></ul>		
BDUR Solver	Specifies the value of the “duration of combustion,” $Dq_c$ , in the Wiebe function. $Dq_c$ must be greater than 0.			
	Parameters	Optional/Reqd.	Units	Examples
	Duration of combustion in number of crank angles	Required	degree	BDUR 45.6
	Keyword Usage	Optional keyword.		
	Reactor Models	<ul style="list-style-type: none"><li>SI Engine Zonal Simulator</li></ul>		
BEFF Solver	Specifies the mass fraction of the fresh fuel-air charge being consumed by the premixed flame, i.e., the combustion efficiency. The combustion efficiency must be $> 0.0$ and $\leq 1.0$ and is set to 1.0 (complete combustion) by default.			
	Parameters	Optional/Reqd.	Units	Examples
	Combustion efficiency	Optional	--	BEFF 0.85
	Keyword Usage	Optional keyword.		
	Reactor Models	<ul style="list-style-type: none"><li>SI Engine Zonal Simulator</li></ul>		
BETA Reactor Property	This is a combined correction factor to the coalescent collision between particles. The van der Waals forces can enhance the collision frequency while non-coalescent collision can reduce the frequency. The default value is 1.0, i.e., van der Waals effect is off and collisions are 100% coalescent.			
	Parameters	Optional/Reqd.	Units	Examples
	Material name	Required	--	BETA <b>C(B)</b> 0.9
	Enhance factor	Required	--	BETA C(B) <b>0.9</b>
	Keyword Usage	Optional keyword.		
	Reactor Models	<ul style="list-style-type: none"><li>Closed Homogeneous Batch Reactor</li><li>Closed Plasma Reactor</li><li>Cylindrical Shear Flow Reactor</li><li>Honeycomb Monolith Reactor</li><li>IC HCCI Engine</li><li>Perfectly Stirred Reactor (PSR)</li></ul>		

Keyword	Definition			
		<ul style="list-style-type: none"><li>Planar Shear Flow Reactor</li><li>Plasma PSR</li><li>Plasma Plug Flow Reactor</li><li>Plug Flow Reactor</li><li>SI Engine Zonal Simulator</li></ul>		
BINI  Solver	Specifies the value of the “duration of combustion,” $q_c$ , in the Wiebe function.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Start of combustion crank angle</i>	Required	degree	BINI -15.3
	Keyword Usage	Optional keyword.		
	Reactor Models	<ul style="list-style-type: none"><li>SI Engine Zonal Simulator</li></ul>		
BLKEQ  Reactor Property	Toggle to turn on or off solution of bulk activities for bulk species.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>String “on” or “off” to turn on or off solution of the bulk-species equations</i>	Required	--	BLKEQ <b>ON</b>  BLKEQ <b>OFF</b>
	Keyword Usage	Optional keyword. By default, bulk-activity equations are solved when there is more than one bulk species in one or more bulk phases on a material. Otherwise the bulk activities are presumed constant at their initial value.		
	Reactor Models	<ul style="list-style-type: none"><li>Closed Homogeneous Batch Reactor</li><li>Closed Plasma Reactor</li><li>Honeycomb Reactor</li><li>Perfectly Stirred Reactor (PSR)</li><li>Plasma Plug Flow Reactor</li><li>Plasma PSR</li><li>Plug Flow Reactor</li></ul>		
BLTK  Reactor Property	Specifies a boundary-layer thickness. When <b>BLTK</b> is declared, a parabolic velocity profile is specified with a zero velocity at each wall increasing to the velocity specified by <b>VEL</b> at a distance of <b>BLTK</b> from the wall. A flat (constant) velocity profile is used for distances greater than <b>BLTK</b> from the wall. In addition, if the initial gas temperature differs from the initial surface temperature the application			



Keyword	Definition			
	linearly interpolates the gas-phase temperature profile between the wall temperature and the bulk gas temperature over the distance <a href="#">BLTK</a> .			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Boundary-layer thickness</i>	Required	cm	BLTK <b>0.05</b>
	<b>Keyword Usage</b>	Optional keyword. By default, the boundary-layer thickness is set to 0 and a full parabolic velocity is assumed.		
	<b>Reactor Models</b>	<ul style="list-style-type: none"><li>• Cylindrical Shear Flow Reactor</li><li>• Planar Shear Flow Reactor</li></ul>		
<b>BP-WR</b>  Reactor Property	RF bias power at a specified material. The energy that the ions gain in the sheath is estimated as this power divided by the total ion current to that material as calculated in the plasma-reactor model. For example, “BPWR material1 200” specifies an applied bias of 200 W to the material boundary, <i>material1</i> . The ion energy gain calculated from the sheath model results in a reduced effective power deposition to the electrons (unless <a href="#">ELSH</a> is also specified), as described in <a href="#">Homogeneous 0-D Reactor Models</a> of the <a href="#">Chemkin-Pro Theory Manual</a> .			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Material name</i>	Optional  If there is no material name than the multiplier applies to all materials.	--	BPWR <b>material1</b> 200 1
	<i>RF bias power</i>	Required	watts	BPWR <b>200</b>
	<i>Reactor number (PSR clusters only)</i>	Optional  If no number is given, the profile described by the first two values is assumed to apply to all reactors	--	BPWR material1 200 <b>1</b>

Keyword	Definition			
		in a cluster.		
	Keyword Usage	Optional keyword. By default, the RF bias power is set to 0.0.		
	Reactor Models	<ul style="list-style-type: none"><li>Closed Plasma Reactor</li><li>Plasma PSR</li><li>Plasma Plug Flow Reactor</li></ul>		
BT-MIN	The minimum value of the Spalding heat transfer number to prevent numerical issues at the beginning of liquid vaporization.			
Reactor Property/Model	Parameters	Optional/Reqd.	Units	Examples
	Spalding heat transfer limit	Required	--	BTMIN <b>0.01</b>
	Keyword Usage	Optional keyword. Default is 0.1		
	Reactor Models	<ul style="list-style-type: none"><li>Direct Injection Diesel Engine Simulator</li></ul>		
BULK	The estimated or initial bulk species activities. This is required input for bulk species in bulk phases that are being etched. For example, BULK Ga(d) 1.0 assigns the estimated activity of 1.0 to the Ga(d) bulk phase species.			
Reactor Property	Parameters	Optional/Reqd.	Units	Examples
	Bulk species name	Required	--	BULK <b>Ga(d)</b> 1.0
	Bulk activity	Required	--	BULK Ga(d) <b>1.0</b>
	Keyword Usage	Required keyword. The bulk activity should be specified for bulk species. By default, the initial or estimated bulk species activities are 0.0.		
	Reactor Models	<ul style="list-style-type: none"><li>Closed Homogeneous Batch Reactor</li><li>Closed Plasma Reactor</li><li>Cylindrical Shear Flow Reactor</li><li>Honeycomb Reactor</li><li>Perfectly Stirred Reactor (PSR)</li><li>Planar Shear Flow Reactor</li><li>Plasma Plug Flow Reactor</li><li>Plasma PSR</li><li>Plug Flow Reactor</li><li>Rotating Disk CVD Reactor</li><li>Stagnation Flow CVD Reactor</li></ul>		

Keyword	Definition			
	<b>Notes</b>	<ul style="list-style-type: none"><li>The sum of all estimated bulk phase activities for each bulk phase <math>n</math> should equal one. If they do not sum to one, they will be normalized to one, and a warning message will be printed in the diagnostic output.</li><li>See also: <a href="#">ETCH</a> keyword.</li><li>Formerly <b>ACT</b> keyword for some reactor models in previous ANSYS Chemkin-Pro versions.</li></ul>		
<b>BURN</b>  Reactor Property	Indicates a burner-stabilized flame problem type, with specified inlet flow rates.			
	<b>Keyword Usage</b>	Required keyword.		
	<b>Reactor Models</b>	<ul style="list-style-type: none"><li>Premixed Laminar Burner-stabilized Flame</li></ul>		
	<b>Notes</b>	<ul style="list-style-type: none"><li>The problem-type can be changed for a restart run.</li><li>See also <a href="#">FREE</a>.</li></ul>		
<b>CAAC</b>  Output	The crank angle at 50% mass burned and is also referred as the anchoring angle. This is one of the three crank angle parameters required to construct the Wiebe function profile that will pass these three crank angles at their corresponding burned mass fractions. By default, this angle marks when half of the original mass is burned. All three crank angles, <a href="#">CASC</a> , <a href="#">CAAC</a> , and <a href="#">CAEC</a> must be provided.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Crankangle at 50% mass burned</i>	Required	degree	<b>CAAC 8.1</b>
	<b>Keyword Usage</b>	Optional keyword.		
	<b>Reactor Models</b>	<ul style="list-style-type: none"><li>SI Engine Zonal Simulator</li></ul>		
<b>CAATQ</b>  Output	Calculates the crank angle for the specified amount of total heat release. The crank angle for 10% and 50% of total heat release will be calculated by default.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Percentage of total heat release</i>	Required	percent	<b>CAATQ 90</b>
	<b>Keyword Usage</b>	Optional keyword.		
	<b>Reactor Models</b>	<ul style="list-style-type: none"><li>IC HCCI Engine</li><li>Multi-Zone HCCI Engine Simulator</li><li>SI Engine Zonal Simulator</li></ul>		
<b>CAEC</b>  Output	The crank angle at 90% mass burned. This is one of the three crank angle parameters required to construct the Wiebe function profile that will pass these three crank angles at their corresponding burned mass fractions. By default, this angle marks when 90% of the original mass is burned. All three crank angles, <a href="#">CASC</a> , <a href="#">CAAC</a> , and <a href="#">CAEC</a> must be provided.			
	Parameters	Optional/Reqd.	Units	Examples

Keyword	Definition			
	<i>Crankangle at 90% mass burned</i>	Required	degree	CAEC 23.0
	Keyword Usage	Optional keyword.		
	Reactor Models	• SI Engine Zonal Simulator		
CAIR  Reactor Property	Model coefficients for the air entrainment mass flow rate model. There are three parameters required for “before ignition”, “after ignition”, and “after reaching wall”, respectively.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Coefficient before ignition</i>	Required	--	CAIR 0.9 0.25 1.0
	<i>Coefficient after ignition</i>	Required	--	CAIR 0.9 0.25 1.0
	<i>Coefficient after wall</i>	Required	--	CAIR 0.9 0.25 1.0
	Keyword Usage	Required keyword. Default: before ignition: 1.0, after ignition: 0.58, after hitting wall: 1.2.		
	Reactor Models	• Direct Injection Diesel Engine Simulator		
CARR  Reactor Property	Specify the named species as the carrier gas. This keyword is used to identify the species in calculating binary diffusion coefficients for tables and for non-dimensionalizations that require a binary diffusion coefficient.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Species name</i>	Optional	--	CARR H2
	<i>Species number</i>	Optional	--	CARR 3
	Keyword Usage	Optional keyword. The default is to use the gas species with the largest mole fraction (from the XBTH input) in the bath-gas composition. If the gas-phase bath-gas composition is not specified, the default is to use the first species in the mechanism.		
	Reactor Models	• Mechanism Analyzer		
CASC  Output	The crank angle at 10% mass burned. This is one of the three crank angle parameters required to construct the Wiebe function profile that will pass these three crank angles at their corresponding burned mass fractions. By default, this angle marks when 10% of the original mass is burned. All three crank angles, CASC , CAAC , and CAEC must be provided.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Crankangle at 10% mass burned</i>	Required	degree	CASC -15.4
	Keyword Usage	Optional keyword.		
	Reactor Models	• SI Engine Zonal Simulator		
CD-CT	Include conduction through the substrate in the energy balance. Inclusion of this keyword requires specification of a substrate thickness ( CNDX). This value is used			

Keyword	Definition			
Reactor Property	only if the disk temperature is being calculated from an energy balance by including keyword <b>RADB</b> . See <a href="#">Equation 14.18</a> of the <a href="#">Chemkin-Pro Theory Manual</a> .			
	Keyword Usage	Optional keyword. By default, conduction through the substrate is not included.		
	Reactor Models	<ul style="list-style-type: none"><li>Rotating Disk CVD Reactor</li><li>Stagnation Flow CVD Reactor</li></ul>		
CDIF	Use central differencing on convective terms in the equations.			
Solver	Keyword Usage	Optional keyword. By default, windward differencing is used.		
	Reactor Models	<ul style="list-style-type: none"><li>Diffusion or Premixed Opposed-flow Flame</li><li>Premixed Laminar Burner-stabilized Flame</li><li>Premixed Laminar Flame-speed Calculation</li></ul>		
CFL Reactor Property	The Courant-Friedrichs-Lewy (CFL) number for the convective process; this parameter limits the fraction of particles whose properties can be set to the inlet conditions per time step.			
	Parameters	Optional/Reqd.	Units	Examples
	CFL number	Required	--	CFL <b>1.0</b>
	Keyword Usage	Optional keyword. By default, the <b>CFL</b> number is 0.5.		
	Reactor Models	<ul style="list-style-type: none"><li>Closed Partially Stirred Reactor (PaSR)</li><li>Partially Stirred Reactor (PaSR)</li></ul>		
CHEM Reactor Property	Specifies that gas-phase chemistry will be included in the calculations.			
	Keyword Usage	Optional keyword. This option is used to reactivate the chemical kinetics if the <b>NOCH</b> option was in effect for the previous calculation for CVD Reactors. For PaSRs, the default is to neglect chemistry and do a mixing calculation only.		
	Reactor Models	<ul style="list-style-type: none"><li>Closed Partially Stirred Reactor (PaSR)</li><li>Partially Stirred Reactor (PaSR)</li><li>Rotating Disk CVD Reactor</li><li>Stagnation Flow CVD Reactor</li></ul>		
CJ Problem Type	Chapman-Jouguet detonation. In this case, H, S, V, and T contain the unburned state and <b>TEST</b> gives the burned temperature estimate.			
	Keyword Usage	Optional keyword. The user must include exactly one problem-type keyword		
	Reactor Models	<ul style="list-style-type: none"><li>Chemical and Phase Equilibrium Calculations</li></ul>		

Keyword	Definition			
CK-TRN  Reactor Property	An option to use the Chemkin-Pro mixture-averaged transport subroutines to evaluate any transport properties (for example, gas viscosity) needed by the reactor models. This option requires a valid transport linking file from pre-processing of the chemistry set, that is, the chemistry set must include the transport data of all gas species.			
	Keyword Usage	Optional keyword.		
	Reactor Models	<ul style="list-style-type: none"><li>• IC HCCI Engine</li><li>• Multi-Zone HCCI Engine Simulator</li><li>• SI Engine Zonal Simulator</li></ul>		
CLSC  Reactor Property	Defines a critical particle class under which the oxidation process starts to affect (reduce) the particle number density. This parameter is only used by the particle burnout model and has no effect on particle formation and growth. The default value is the minimum particle class plus the maximum class change due to surface reaction.			
	Parameters	Optional/Reqd.	Units	Examples
	Material name	Required	--	CLSC <b>CARBON 40</b>
	Critical particle class	Required	--	CLSC CARBON <b>40</b>
	Keyword Usage	Optional keyword. The default value is the minimum particle class plus the maximum class change due to surface reaction.		
	Reactor Models	<ul style="list-style-type: none"><li>• Closed Homogeneous Batch Reactor</li><li>• Closed Plasma Reactor</li><li>• Cylindrical Shear Flow Reactor</li><li>• Honeycomb Monolith Reactor</li><li>• IC HCCI Engine</li><li>• Perfectly Stirred Reactor (PSR)</li><li>• Planar Shear Flow Reactor</li><li>• Plasma PSR</li><li>• Plasma Plug Flow Reactor</li><li>• Plug Flow Reactor</li><li>• SI Engine Zonal Simulator</li></ul>		
CLSE  Reactor Property	Flag indicating the reactor is a closed system, i.e., mass flow rate is zero.			
	Keyword Usage	Required Keyword.		
	Reactor Models	<ul style="list-style-type: none"><li>• Closed Partially Stirred Reactor (PaSR)</li></ul>		

Keyword	Definition			
CLSM  Reactor Property	Defines the smallest particle class that can exist in the system. This parameter is only used by the particle burnout model and has no effect on particle formation and growth. The default value is the smallest inception class defined by the nucleation reactions.			
	Parameters	Optional/Reqd.	Units	Examples
	Material name	Required	--	CLSM <b>CARBON 32</b>
	Minimum particle class	Required	--	CLSM CARBON <b>32</b>
	Keyword Usage	Optional keyword. The default value is the smallest inception class defined by the nucleation reactions.		
	Reactor Models	<ul style="list-style-type: none"><li>• Closed Homogeneous Batch Reactor</li><li>• Closed Plasma Reactor</li><li>• Cylindrical Shear Flow Reactor</li><li>• Honeycomb Monolith Reactor</li><li>• IC HCCI Engine</li><li>• Perfectly Stirred Reactor (PSR)</li><li>• Planar Shear Flow Reactor</li><li>• Plasma PSR</li><li>• Plasma Plug Flow Reactor</li><li>• Plug Flow Reactor</li><li>• SI Engine Zonal Simulator</li></ul>		
CMIX  Reactor Property	The controlling parameter for the modified Curl's and the <a href="#">IEM</a> models for a PaSR.			
	Parameters	Optional/Reqd.	Units	Examples
	Time ratio for scalar mixing ( <a href="#">Equation 9.1</a> of the <a href="#">Chemkin-Pro Theory Manual</a> )	Required	--	CMIX <b>1.0</b>
	Keyword Usage	Required keyword, unless <a href="#">WELL</a> keyword is included.		
	Reactor Models	<ul style="list-style-type: none"><li>• Closed Partially Stirred Reactor (PaSR)</li><li>• Partially Stirred Reactor (PaSR)</li></ul>		
CM-PR  Reactor Property	Engine compression ratio. The compression ratio is defined as the maximum total volume in the cylinder (clearance volume plus swept volume) divided by the clearance volume.			
	Parameters	Optional/Reqd.	Units	Examples

Keyword	Definition			
	<i>Engine compression ratio</i>	Required	--	CMPR <b>10</b>
	<b>Keyword Usage</b>	Optional keyword. By default, the ratio is 15.		
	<b>Reactor Models</b>	<ul style="list-style-type: none"><li>• IC HCCI Engine</li><li>• SI Engine Zonal Simulator</li></ul>		
<b>CNDT</b> Reactor Property	The back-side temperature of the substrate for use in calculation of conduction losses. This value is used only if the disk temperature is being calculated from an energy balance by including keywords <a href="#">RADB</a> and <a href="#">CDCT</a> . See <a href="#">Equation 14.18</a> of the <a href="#">Chemkin-Pro Theory Manual</a> .			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Back-side temperature</i>	Required	K	CNDT <b>350.</b>
	<b>Keyword Usage</b>	Optional keyword. By default, the back-side temperature is 300.		
	<b>Reactor Models</b>	<ul style="list-style-type: none"><li>• Rotating Disk CVD Reactor</li><li>• Stagnation Flow CVD Reactor</li></ul>		
<b>CNDX</b> Reactor Property	The thickness of the substrate for calculation of conduction losses. This value is used only if the disk temperature is being calculated from an energy balance by including keywords <a href="#">RADB</a> and <a href="#">CDCT</a> . See <a href="#">Equation 14.18</a> of the <a href="#">Chemkin-Pro Theory Manual</a> .			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Substrate thickness</i>	Required	cm	CNDX <b>0.03</b>
	<b>Keyword Usage</b>	Optional keyword. By default, the substrate thickness is 0.0.		
	<b>Reactor Models</b>	<ul style="list-style-type: none"><li>• Rotating Disk CVD Reactor</li><li>• Stagnation Flow CVD Reactor</li></ul>		
<b>CNTN</b> Reactor Property	Inclusion of this keyword causes ANSYS Chemkin-Pro to expect keywords for another problem to follow the <a href="#">END</a> keyword. The following problem uses the solution of the previous problem as its initial guess. This capability is very similar to that provided by <a href="#">RSTR</a> . However, in the case of <a href="#">CNTN</a> , several related problems can be solved by one job submission, without having to manipulate the XML Solution File. The solutions resulting from <a href="#">CNTN</a> keywords are written sequentially to one XML Solution File.			
	<b>Keyword Usage</b>	Optional keyword. By default, no continuation is expected.		
	<b>Reactor Models</b>	<ul style="list-style-type: none"><li>• Closed Homogeneous Batch Reactor</li><li>• Closed Plasma Reactor</li><li>• Cylindrical Shear Flow Reactor</li></ul>		



Keyword	Definition	
		<ul style="list-style-type: none"> <li>• Honeycomb Reactor</li> <li>• IC HCCI Engine</li> <li>• Non-reactive Gas Mixer</li> <li>• Normal Incident Shock</li> <li>• Normal Reflected Shock</li> <li>• Opposed-flow Flame Simulator</li> <li>• Perfectly Stirred Reactor (PSR)</li> <li>• Planar Shear Flow Reactor</li> <li>• Plasma Plug Flow Reactor</li> <li>• Plasma PSR</li> <li>• Plug Flow Reactor</li> <li>• Premixed Laminar Burner-stabilized Flame</li> <li>• Premixed Laminar Flame-speed Calculation</li> <li>• Rotating Disk CVD Reactor Using Steady-state Solver</li> <li>• SI Engine Zonal Simulator</li> <li>• Stagnation Flow CVD Reactor Using Steady-state Solver</li> </ul>
<b>CNTT</b>  Reactor Property	This will cause the starting time of the continuation calculation to be equal to the end time of the last solution.	
	<b>Keyword Usage</b>	Optional keyword. By default, the starting time of a continuation is set to zero.
	<b>Reactor Models</b>	<ul style="list-style-type: none"> <li>• Closed Homogeneous Batch Reactor</li> <li>• Closed Plasma Reactor</li> <li>• IC HCCI Engine</li> <li>• Non-reactive Gas Mixer</li> <li>• Perfectly Stirred Reactor (PSR)</li> <li>• Plasma PSR</li> <li>• SI Engine Zonal Simulator</li> </ul>
<b>CNTX</b>	This will cause the starting distance of the continuation calculation to be equal to the end distance of the last solution. This keyword is used for Plug Flow Reactors in place of <a href="#">CNTT</a> .	

Keyword	Definition			
Reactor Property	Keyword Usage	Optional keyword. By default, the starting distance of a continuation is set to zero.		
	Reactor Models	<ul style="list-style-type: none"><li>• Honeycomb Reactor</li><li>• Plasma Plug Flow Reactor</li><li>• Plug Flow Reactor</li></ul>		
COLR Reactor Property	This flag indicates the collision formulation to be used to calculate the collision rate among particles. Three types of collision formulations are available: free molecular regime (=0), continuum regime (=1), and transition regime (=3). The collision rate in the transition regime is obtained as the harmonic mean of the collision rates of free-molecular regime and continuum regime. By default, formulation for free-molecular collision is used.			
	Parameters	Optional/Reqd.	Units	Examples
	Material name	Required	--	COLR <b>C(B)</b> 1
	Collision regime	Required	--	BETA C(B) <b>1</b>
	Keyword Usage	Optional keyword. By default, the formulation for the free-molecular regime is used (0).		
	Reactor Models	<ul style="list-style-type: none"><li>• Closed Homogeneous Batch Reactor</li><li>• Closed Plasma Reactor</li><li>• Cylindrical Shear Flow Reactor</li><li>• Honeycomb Monolith Reactor</li><li>• IC HCCI Engine</li><li>• Perfectly Stirred Reactor (PSR)</li><li>• Planar Shear Flow Reactor</li><li>• Plasma PSR</li><li>• Plasma Plug Flow Reactor</li><li>• Plug Flow Reactor</li><li>• SI Engine Zonal Simulator</li></ul>		
COMP Reactor Property	The boundary condition used at the inlet boundary for the gas species equations will be that of a fixed gas composition, as specified by the REAC keywords.			
	Keyword Usage	Optional keyword. By default, a flux balance is solved at the inlet (see keyword FLUX).		
	Reactor Models	<ul style="list-style-type: none"><li>• Rotating Disk CVD Reactor</li><li>• Stagnation Flow CVD Reactor</li></ul>		

Keyword	Definition			
CONC Output	If this keyword is used, the printed output will appear in molar concentration (mole/cc) rather than mole fraction.			
	Keyword Usage	Optional keyword. By default, mole fractions are printed.		
	Reactions	<ul style="list-style-type: none"><li>• Normal Incident Shock</li><li>• Normal Reflected Shock</li></ul>		
COND Reactor Property	The thermal conductivity of the substrate in SI units, for use in calculation of conduction losses. This value is used only if the disk temperature is being calculated from an energy balance by including keywords RADB and CDCT . See Equation 14.18 of the Chemkin-Pro Theory Manual .			
	Parameters	Optional/Reqd.	Units	Examples
	Thermal conductivity	Required	W/cm K	COND 2.1
	Keyword Usage	Optional keyword. By default, the thermal conductivity is 1.38.		
	Reactor Models	<ul style="list-style-type: none"><li>• Rotating Disk CVD Reactor</li><li>• Stagnation Flow CVD Reactor</li></ul>		
CONP Problem Type	A transient solution will be obtained with the pressure held constant. The equations solved are those of a constant pressuresystem and the energy equation will be solved.			
	Keyword Usage	Optional keyword. By default, a constant pressure problem is assumed.		
	Reactor Models	<ul style="list-style-type: none"><li>• Closed Homogeneous Batch Reactor</li><li>• Closed Plasma Reactor</li></ul>		
CONV Problem Type	A transient solution will be obtained with the volume held constant. The equations solved are those of a constant volume system and the energy equation will be solved. In this case, the pressure is allowed to float.			
	Keyword Usage	Optional keyword. By default, a constant pressure problem is assumed.		
	Reactor Models	<ul style="list-style-type: none"><li>• Closed Homogeneous Batch Reactor</li><li>• Closed Plasma Reactor</li></ul>		
CONX Reactor Property	This keyword is used to specify a constant (constrained) mole fraction for a species. For example, CONX H2 0.1 will fix the fraction of hydrogen in the mixture to be 0.1.			
	Parameters	Optional/Reqd.	Units	Examples
	Species name	Required	--	CONX H20.1
	Mole fraction of the species	Required	mole fraction	CONX H2 0.1

Keyword	Definition			
	<b>Keyword Usage</b>	Optional keyword. By default, composition equilibrium is determined for all species.		
	<b>Reactor Models</b>	• Chemical and Phase Equilibrium Calculations		
<b>COTV</b>  Problem Type	• A transient solution will be obtained with the  • temperature and  • volume held  • constant at the initial values. In this case, the pressure is allowed to float.			
	<b>Keyword Usage</b>	Optional keyword. By default, a constant pressure is assumed.		
	<b>Reactor Models</b>	• Closed Homogeneous Batch Reactor		
<b>CPROD</b>  Inlet or Reactor Property	One of these <b>CPROD</b> inputs must appear for each complete-combustion product species when the equivalence ratio option is used ( <b>EQUI</b> ) for an inlet stream or for the initial conditions of a closed system.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Inlet stream name (PSRs only)</i>	Optional  If there is no stream name than the product species will be used for all defined inlet streams.	--	CPROD <b>mixture1</b> CO2  CPROD <b>mixture1</b> H2O
	<i>Species name</i>	Required	--	CPROD H2OCPROD <b>CO2</b>
	<b>Keyword Usage</b>	Required keyword when <b>EQUI</b> option is used for an inlet stream or for the initial conditions in a reactor. The specified group of complete-combustion product species must include all of the elements contained in the fuel and oxidizer species. The products must also be “saturated” species. See the ANSYS Chemkin-Pro Tutorials Manual for more information.		
	<b>Reactor Models</b>	• Chemical and Phase Equilibrium Calculations  • Closed Homogeneous Batch Reactor  • Closed Plasma Reactor		

Keyword	Definition			
		<ul style="list-style-type: none"><li>• Cylindrical Shear Flow Reactor</li><li>• Diffusion or Premixed Opposed-flow Flame</li><li>• Honeycomb Reactor</li><li>• IC HCCI Engine</li><li>• Non-reactive Gas Mixer</li><li>• Partially Stirred Reactor (PaSR)</li><li>• Perfectly Stirred Reactor (PSR)</li><li>• Planar Shear Flow Reactor</li><li>• Plasma Plug Flow Reactor</li><li>• Plasma PSR</li><li>• Plug Flow Reactor</li><li>• Premixed Laminar Burner-stabilized Flame</li><li>• Premixed Laminar Flame-speed Calculation</li><li>• Rotating Disk CVD Reactor</li><li>• Stagnation Flow CVD Reactor</li></ul>		
	Notes	<ul style="list-style-type: none"><li>• The CPROD keywords must be changed as a set, not individually for a restart run.</li><li>• The CPROD keywords must be changed as a set, not individually for continuation run.</li></ul>		
CTOL  Reactor Property	Criterion for determining when steady state is reached using a transient solver for Partially Stirred Reactors. The required parameter sets the normalized slope of mean density change in time $\left(d\bar{p}/dt\right)$ . The default number of time points used to determine the slope is 100; this value can be changed with the keyword NCFIT.			
	Parameters	Optional/Reqd.	Units	Examples
	Normalized slope of mean density	Required	--	CTOL <b>1.0E-3</b>
	Keyword Usage	Optional keyword. By default, the program does not check for the steady state.		
	Reactor Models	<ul style="list-style-type: none"><li>• Closed Partially Stirred Reactor (PaSR)</li><li>• Partially Stirred Reactor (PaSR)</li></ul>		

Keyword	Definition			
CTOL Solver	Criterion for determining when steady-state is reached by a transient solver for CVD Reactors. The steady state is reached when the normalized absolute values of all time derivatives are less than CTOL.			
	Parameters	Optional/Reqd.	Units	Examples
	Steady-state criterion	Required	--	CTOL <b>1.0E-2</b>
	Keyword Usage	Optional keyword. By default, the criterion is 1.0E-4.		
	Reactor Models	<ul style="list-style-type: none"><li>Rotating Disk CVD Reactor</li><li>Stagnation Flow CVD Reactor</li></ul>		
CURL Reactor Property	Flag indicating that the modified Curl's model will be used to simulate the molecular mixing within the computational particle.			
	Keyword Usage	Optional keyword. By default, a well mixed model is assumed.		
	Reactor Models	<ul style="list-style-type: none"><li>Closed Partially Stirred Reactor (PaSR)</li><li>Partially Stirred Reactor (PaSR)</li></ul>		
CURV Solver	Parameter that controls the degree of mesh adaptation based on the second derivative, or curvature, in the solution. A reasonable value is usually between about 0.1 and 1.0, where no adaptation based on curvature is specified with 1.0.			
	Parameters	Optional/Reqd.	Units	Examples
	Normalized curvature parameter	Required	--	CURV <b>0.7</b>
	Keyword Usage	Optional keyword. By default, the curvature parameter is set to 0.5.		
	Reactor Models	<ul style="list-style-type: none"><li>Diffusion or Premixed Opposed-flow Flame</li><li>Premixed Laminar Burner-stabilized Flame</li><li>Premixed Laminar Flame-speed Calculation</li><li>Rotating Disk CVD Reactor</li><li>Stagnation Flow CVD Reactor</li></ul>		
	Notes	<ul style="list-style-type: none"><li>This keyword can be changed for a restart run.</li><li><a href="#">Steady-state 1-D Solution Methods</a> of the <a href="#">Chemkin-Pro Theory Manual</a> for more information.</li></ul>		
CY-BAR Reactor Property	The cylinder head area to bore-area ratio.			
	Parameters	Optional/Reqd.	Units	Examples

Keyword	Definition			
	<i>Ratio of cylinder head area to bore area.</i>	Required	None	CYBAR <b>1.2</b>
	<b>Keyword Usage</b>	Optional keyword. Default = 1.0.		
	<b>Reactor Models</b>	<ul style="list-style-type: none"><li>• IC HCCI Engine</li><li>• Multi-zone HCCI Engine</li><li>• SI Engine Zonal Simulator</li></ul>		
	<b>Notes</b>	<ul style="list-style-type: none"><li>• CYBAR should be &gt; 1.0.</li></ul>		
<b>DASP</b>  Solver	Flag indicating the DASPK solver is used to integrate the transient equations.			
	<b>Keyword Usage</b>	Optional keyword. By default, the DASPK solver will be used.		
	<b>Reactor Models</b>	<ul style="list-style-type: none"><li>• Closed Partially Stirred Reactor (PaSR)</li><li>• Partially Stirred Reactor (PaSR)</li></ul>		
<b>DEGO</b>  Reactor Property	The starting crank angle for the transient IC HCCI Engine model, in degrees.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Crank angle</i>	Required	degrees	DEGO <b>45</b>
	<b>Keyword Usage</b>	Optional keyword. By default, this starting angle is 180 degrees.		
	<b>Reactor Models</b>	<ul style="list-style-type: none"><li>• IC HCCI Engine</li><li>• SI Engine Zonal Simulator</li></ul>		
<b>DE-GE</b>  Output	The ending crank angle for the IC engine simulation. Normally, this is the same as the crank angle at Exhaust Valve Open (EVO).			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Crankangle at end of simulation</i>	Required	degree	<b>CAAC 120.5</b>
	<b>Keyword Usage</b>	Optional keyword.		
	<b>Reactor Models</b>	<ul style="list-style-type: none"><li>• IC HCCI Engine</li><li>• Multi-zone HCCI Engine</li><li>• SI Engine Zonal Simulator</li></ul>		
<b>DELT</b>  Solver	The time interval for solution printing to the diagnostic text output file, for the transient solver. Note that the number of time points written to the diagnostic output file is equal to the value given by <b>TIME</b> divided by <b>DELT</b> .			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Time interval</i>	Required	sec	DELT <b>1.0E-4</b>

Keyword	Definition			
	<i>Aurora Usage</i>	Optional keyword. By default, the value of the maximum solver timestep ( <i>STPT</i> ) is used.		
	<i>Spin Usage</i>	Optional keyword. By default, this is a required keyword for a transient calculation.		
	<b>Reactor Models</b>	<ul style="list-style-type: none"><li>• Closed Homogeneous Batch Reactor</li><li>• Closed Plasma Reactor</li><li>• IC HCCI Engine</li><li>• Non-reactive Gas Mixer</li><li>• Normal Incident Shock</li><li>• Normal Reflected Shock</li><li>• Perfectly Stirred Reactor (PSR)</li><li>• Plasma PSR</li><li>• Rotating Disk CVD Reactor</li><li>• Stagnation Flow CVD Reactor</li><li>• SI Engine Zonal Simulator</li></ul>		
	<b>Notes</b>	• Backwards compatible with <b>DT</b> from previous versions.		
<b>DFAC</b>  Solver	Factor by which to divide the time step in the steady-state solver, <i>Twopnt's</i> , time stepping procedure when necessary, i.e., when the current time step does not converge.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Division factor</i>	Required	--	DFAC <b>1.5</b>
	<b>Keyword Usage</b>	Optional keyword. By default, the division factor is set to 2.2.		
	<b>Reactor Models</b>	<ul style="list-style-type: none"><li>• Closed Plasma Reactor</li><li>• Diffusion or Premixed Opposed-flow Flame</li><li>• Non-reactive Gas Mixer</li><li>• Perfectly Stirred Reactor (PSR)</li><li>• Plasma PSR</li><li>• Premixed Laminar Burner-stabilized Flame</li><li>• Premixed Laminar Flame-speed Calculation</li><li>• Rotating Disk CVD Reactor</li></ul>		



Keyword	Definition			
		• Stagnation Flow CVD Reactor		
DIA  Reactor Property	Shock-tube diameter, used for boundary layer corrections.			
	Parameters	Optional/Reqd.	Units	Examples
	Tube diameter	Required	cm	DIA <b>2.0</b>
	Keyword Usage	Optional keyword. By default, the tube diameter is set to 1.0.		
	Reactor Models	• Normal Incident Shock		
DIAM  Reactor Property	Tube diameter or hydraulic diameter, where the diameter is constant along the channel. See also <a href="#">DPRO</a> , <a href="#">AREAF</a> , <a href="#">AFLO</a> and user subroutine GEOM.			
	Parameters	Optional/Reqd.	Units	Examples
	Tube diameter	Required	cm	DIAM <b>5.3</b>
	Keyword Usage	Optional keyword. The user must specify <a href="#">DIAM</a> , <a href="#">DPRO</a> , <a href="#">AREAF</a> , or <a href="#">AFLO</a> , unless the GEOM user routine is to be used.		
	Reactor Models	• Honeycomb Reactor  • Plasma Plug Flow Reactor  • Plug Flow Reactor		
DI-EN  Problem Type	Specify that the spray-Combustion Direct Injection Engine Model is used. The <a href="#">???</a> keyword must also be included in the same input file.			
	Keyword Usage	Required keyword.		
	Reactor Models	• Direct Injection Diesel Engine Simulator		
DIN-ZL  Inlet Property	Define the name of the injector.			
	Parameters	Optional/Reqd.	Units	Examples
	Name of injector	Required	--	DINZL <b>modelX</b>
	Keyword Usage	Required keyword.		
	Reactor Models	• Direct Injection Diesel Engine Simulator		
DIST  XMLI	This keyword is valid with the <a href="#">XMLI</a> option, when the XML Solution File that is used for initialization or restart contains data as a function of axial distance (e.g. from Shear-layer Flow or Plug Flow). In this case, select the values to use in initialization or restart as those corresponding to the distance that is closest to (greater than or equal to) the specified distance.			
	Parameters	Optional/Reqd.	Units	Examples
	Axial distance	Required	cm	DIST <b>5.0</b>
	Keyword Usage	Optional keyword. By default, uses the data from the last axial distance found in the XML Solution File.		
	Reactor Models	• Chemical and Phase Equilibrium Calculations  • Closed Homogeneous Batch Reactor		

Keyword	Definition			
	<ul style="list-style-type: none"> <li>• Closed Plasma Reactor</li> <li>• Cylindrical Shear Flow Reactor</li> <li>• Diffusion or Premixed Opposed-flow Flame</li> <li>• Honeycomb Reactor</li> <li>• IC HCCI Engine</li> <li>• Mechanism Analyzer</li> <li>• Non-reactive Gas Mixer</li> <li>• Normal Incident Shock</li> <li>• Normal Reflected Shock</li> <li>• Perfectly Stirred Reactor (PSR)</li> <li>• Planar Shear Flow Reactor</li> <li>• Plasma Plug Flow Reactor</li> <li>• Plasma PSR</li> <li>• Plug Flow Reactor</li> <li>• Premixed Laminar Burner-stabilized Flame</li> <li>• Premixed Laminar Flame-speed Calculation</li> <li>• Rotating Disk CVD Reactor</li> <li>• SI Engine Zonal Simulator</li> <li>• Stagnation Flow CVD Reactor</li> </ul>			
<b>DPRO</b>  Reactor Property Profiles	Hydraulic diameter or tube diameter as a function of distance. See also <a href="#">DIAM</a> , <a href="#">AREAF</a> , <a href="#">AFLO</a> , and user subroutine GEOM.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Distance from inlet</i>	Required	cm	DPRO <b>0.01.0</b>
	<i>Hydraulic diameter</i>	Required	cm	DPRO 0.0 <b>1.0</b>
	<b>Keyword Usage</b>	Optional keyword. The user must enter <a href="#">DIAM</a> , <a href="#">DPRO</a> , <a href="#">AREAF</a> , or <a href="#">AFLO</a> , unless user subroutine GEOM is to be used.		
	<b>Reactor Models</b>	<ul style="list-style-type: none"> <li>• Honeycomb Reactor</li> <li>• Plasma Plug Flow Reactor</li> <li>• Plug Flow Reactor</li> </ul>		

Keyword	Definition			
<b>DT</b>  Reactor Property	The time step size of the Monte Carlo simulation.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Time step</i>	Required	sec	DT <b>1.0E-4</b>
	<b>Keyword Usage</b>	Required keyword.		
	<b>Reactor Models</b>	<ul style="list-style-type: none"><li>• Closed Partially Stirred Reactor (PaSR)</li><li>• Partially Stirred Reactor (PaSR)</li></ul>		
<b>DT0</b>  Solver	The initial time step size used by the transient solver.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Initial time step size</i>	Required	sec	DT0 <b>1.0E-4</b>
	<b>Keyword Usage</b>	Optional keyword. By default, the initial time step size is set to 1.0E-6.		
	<b>Reactor Models</b>	<ul style="list-style-type: none"><li>• Closed Partially Stirred Reactor (PaSR)</li><li>• Partially Stirred Reactor (PaSR)</li><li>• Rotating Disk CVD Reactor</li><li>• Stagnation Flow CVD Reactor</li></ul>		
	<b>Notes</b>	<ul style="list-style-type: none"><li>• Backwards compatible with <a href="#">H0</a> keyword.</li></ul>		
<b>DTDEG</b>  Solver	The maximum time step in terms of crank angle that may be taken by the DASPK solver for the transient IC HCCI Engine model, in degrees. If <a href="#">DTDEG</a> is specified, then it will overwrite the time step value specified by <a href="#">STPT</a> .			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Time step</i>	Required	degrees	DTDEG <b>30</b>
	<b>Keyword Usage</b>	Optional keyword. By default, this time step is value of <a href="#">STPT</a> .		
	<b>Reactor Models</b>	<ul style="list-style-type: none"><li>• IC HCCI Engine</li><li>• SI Engine Zonal Simulator</li></ul>		
	<b>Notes</b>	<ul style="list-style-type: none"><li>• See also: <a href="#">STPT</a> keyword.</li></ul>		
<b>DTIGN</b>  Output	Temperature threshold used to determine when ignition has occurred and allow printing of ignition delay times. The ignition temperature will be the initial temperature plus this value. Only applicable when you are solving the energy equation with the transient solver.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Ignition temperature delta</i>	Required	K	DTIGN <b>200</b>
	<b>Keyword Usage</b>	Optional keyword. See also <a href="#">TLIM</a> .		
	<b>Reactor Models</b>	<ul style="list-style-type: none"><li>• Closed Homogeneous Batch Reactor</li></ul>		

Keyword	Definition			
		<ul style="list-style-type: none"><li>• Closed Plasma Reactor</li><li>• Honeycomb Monolith Reactor</li><li>• IC HCCI Engine</li><li>• Perfectly Stirred Reactor (PSR)</li><li>• Plasma PSR</li><li>• Plasma Plug Flow Reactor</li><li>• Plug Flow Reactor</li><li>• SI Engine Zonal Simulator</li></ul>		
DTMN Solver	Minimum time step tolerated in the steady-state solver, <i>Twopnt</i> 's time stepping algorithm before flagging an error condition.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Minimum time step</i>	Required	sec	DTMN <b>1.E-9</b>
	Keyword Usage	Optional keyword. By default, the minimum time step is 1.E-10.		
	Reactor Models	<ul style="list-style-type: none"><li>• Cylindrical Shear Flow Reactor</li><li>• Diffusion or Premixed Opposed-flow Flame</li><li>• Non-reactive Gas Mixer</li><li>• Perfectly Stirred Reactor (PSR)</li><li>• Plasma PSR</li><li>• Rotating Disk CVD Reactor</li><li>• Stagnation Flow CVD Reactor</li><li>• Planar Shear Flow Reactor</li><li>• Premixed Laminar Burner-stabilized Flame</li><li>• Premixed Laminar Flame-speed Calculation</li></ul>		
DTMX (steady-state) Solver	Maximum time step allowed in <i>Twopnt</i> 's time-stepping algorithm. When this value is reached, the time step size will no longer be increased and time stepping will continue with a fixed time step.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Maximum time step</i>	Required	sec	DTMX <b>1.E-3</b>
	Keyword Usage	Optional keyword. By default, the maximum time step is 1.E-2.		
	Reactor Models	<ul style="list-style-type: none"><li>• Cylindrical Shear Flow Reactor</li></ul>		

Keyword	Definition			
		<ul style="list-style-type: none"><li>• Diffusion or Premixed Opposed-flow Flame</li><li>• Non-reactive Gas Mixer</li><li>• Perfectly Stirred Reactor (PSR)</li><li>• Planar Shear Flow Reactor</li><li>• Plasma PSR</li><li>• Premixed Laminar Burner-stabilized Flame</li><li>• Premixed Laminar Flame-speed Calculation</li><li>• Rotating Disk CVD Reactor</li><li>• Stagnation Flow CVD Reactor</li></ul>		
<b>DTMX</b>  (transient) Solver	Maximum time step used internally by the solver in transient calculations. <a href="#">DTMX</a> determines the largest time-step the transient solver can take at one time and thereby controls the resolution for interpolation of specified time-profiles.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Maximum time step</i>	Required	sec	DTMX <b>1.E-3</b>
	<b>Keyword Usage</b>	Optional keyword. By default, the maximum time step is 1.E-4.		
	<b>Reactor Models</b>	<ul style="list-style-type: none"><li>• Closed Partially Stirred Reactor (PaSR)</li><li>• Partially Stirred Reactor (PaSR)</li></ul>		
<b>DTSV</b>  Output or Solver	Controls the time interval for data to be written to the XML Solution File (e.g., <i>XMLdata.zip</i> ). Note that the number of time points written to the XML Solution File is equal to the value given by <a href="#">TIME</a> divided by <a href="#">DTSV</a> .			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Time interval for solution saving</i>	Required	sec	DTSV <b>1.0E-5</b>
	<b>Keyword Usage</b>	Optional keyword. By default, the value of the <a href="#">STPT</a> keyword is used.		
	<b>Reactor Models</b>	<ul style="list-style-type: none"><li>• Closed Homogeneous Batch Reactor</li><li>• Closed Plasma Reactor</li><li>• IC HCCI Engine</li><li>• Non-reactive Gas Mixer</li><li>• Perfectly Stirred Reactor (PSR)</li><li>• Plasma PSR</li><li>• Closed Partially Stirred Reactor (PaSR)</li></ul>		

Keyword	Definition			
		<ul style="list-style-type: none"><li>Partially Stirred Reactor (PaSR)</li><li>SI Engine Zonal Simulator</li></ul>		
DX  Output or Solver	Distance interval for printing the solution to the diagnostic output file.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Distance interval</i>	Required	cm	DX <b>0.25.</b>
	<b>Keyword Usage</b>	Optional keyword. By default, the distance interval is the value of the <b>DXMX</b> is used, or <b>XEND</b> divided by 100 if <b>DXMX</b> is not available.		
	<b>Reactor Models</b>	<ul style="list-style-type: none"><li>Cylindrical Shear Flow Reactor</li><li>Honeycomb Reactor</li><li>Planar Shear Flow Reactor</li><li>Plasma Plug Flow Reactor</li><li>Plug Flow Reactor</li></ul>		
DXMX  Solver	The maximum distance step that can be used internally by the transient solver. <b>DXMX</b> determines the largest step that the solver can take at one time and thereby controls the resolution for interpolation of specified spatial-profiles. See also <b>DX</b> and <b>DXSV</b> .			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Distance interval</i>	Required	cm	DXMX <b>0.1</b>
	<b>Keyword Usage</b>	Optional keyword. By default, If either <b>DX</b> or <b>DXSV</b> are specified, then <b>DXMX</b> is set to the smallest of these values. If neither <b>DX</b> nor <b>DXSV</b> are specified, then <b>DXMX</b> is set to the value of <b>XEND</b> divided by 100.		
	<b>Reactor Models</b>	<ul style="list-style-type: none"><li>Cylindrical Shear Flow Reactor</li><li>Honeycomb Reactor</li><li>Planar Shear Flow Reactor</li><li>Plasma Plug Flow Reactor</li><li>Plug Flow Reactor</li></ul>		
DXSV  Solver	Controls the distance interval for data to be written to the XML Solution File (e.g., <i>XMLdata.zip</i> ). The number of points written to the XML Solution File is equal to the value given by <b>XEND</b> divided by <b>DXSV</b> .			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Distance interval</i>	Required	cm	DXSV <b>0.1</b>
	<b>Keyword Usage</b>	Optional keyword. By default, the value of <b>DXMX</b> is used.		
	<b>Reactor Models</b>	<ul style="list-style-type: none"><li>Cylindrical Shear Flow Reactor</li></ul>		

Keyword	Definition			
		<ul style="list-style-type: none"><li>• Honeycomb Reactor</li><li>• Planar Shear Flow Reactor</li><li>• Plasma Plug Flow Reactor</li><li>• Plug Flow Reactor</li></ul>		
EGRR  Reactor or Inlet Property	Specifies the EGR rate for an inlet stream or for the initial conditions in a closed reactor.			
	Parameters	Optional/Reqd.	Units	Examples
	EGR ratio	Optional	None	EGRR <b>0.2</b>
	Keyword Usage	Optional keyword. EGR rate can be used in any reactor model as a feature on input or initial composition panels. EGR specification can be activated when Equivalence ratio option is used to specify inlet or initial composition. Leaving the EGR Rate box empty will use no EGR, but use diluants if specified on the Added Species tab. When EGR Rate is specified, the composition on the Added Species tab is used as the EGR composition. The sum of all the fractions on the Added Species tab should be 1.0 when EGR Rate is specified. If the sum is less than 1, Chemkin will automatically normalize the EGR composition.		
	Reactor Models	<ul style="list-style-type: none"><li>• Closed Homogeneous Batch Reactor</li><li>• IC HCCI Engine</li><li>• Perfectly Stirred Reactor (PSR)</li><li>• Honeycomb Reactor</li><li>• Plasma Plug Flow Reactor</li><li>• Plasma PSR</li><li>• Plug Flow Reactor</li></ul>		
ELSH  Reactor Property	Specified energy loss to ions in the sheath for each ion lost at a specified material. The energy that the ions gain in the sheath is typically assumed to be the sheath voltage, which can be described as a multiplier of $kT_e$ . The value given here is the value of the multiplier. For example, "ELSH material1 5.0" would result in an ion energy gain of $5kT_e$ as it crossed the sheath near the material material1. This energy gain for the ions results in a reduced effective power deposition to the electrons, as described in <a href="#">Plasma Systems</a> of the <a href="#">Chemkin-Pro Theory Manual</a> .			
	Parameters	Optional/Reqd.	Units	Examples
	Material name	Optional  If there is no	--	ELSH <b>material1</b> 5.0 1

Keyword	Definition			
		material name then the multiplier applies to all materials.		
	Multiplier value	Required	--	ELSH <b>5.0</b>
	Reactor number (PSR clusters only)	Optional  If no number is given, values are assumed to apply to all reactors in a cluster.	--	ELSH material1 5.0 <b>1</b>
	Keyword Usage	Optional keyword. By default, the multiplier is set to 0.0, when no <a href="#">ELSH</a> keyword is included.		
	Reactor Models	<ul style="list-style-type: none"><li>• Closed Plasma Reactor</li><li>• Plasma Plug Flow Reactor</li><li>• Plasma PSR</li></ul>		
EMIS  Reactor Property	The emissivity of the disk. This value is used only if the disk temperature is being calculated from an energy balance by including keyword <a href="#">RADB</a> . See <a href="#">Equation 14.18</a> of the <a href="#">Chemkin-Pro Theory Manual</a> .			
	Parameters	Optional/Reqd.	Units	Examples
	Emissivity	Required	--	EMIS <b>0.9</b>
	Keyword Usage	Optional keyword. By default, the emissivity is 0.85.		
	Reactor Models	<ul style="list-style-type: none"><li>• Rotating Disk CVD Reactor</li><li>• Stagnation Flow CVD Reactor</li></ul>		
EM-PAR  Reactor Property	This keyword provides the value of the model parameter $C_{\text{part}}$ for computing the overall emissivity of the named particle cloud as given in <a href="#">Equation 12.21</a> in the <a href="#">Chemkin-Pro Theory Manual</a> .			
	Parameters	Optional/Reqd.	Units	Examples
	Material name	Required	--	EMPAR soot 700
	Model coefficient	Required	$\text{m}^{-1}\text{K}^{-1}$	EMPAR soot <b>700</b>
	Keyword Usage	Optional keyword. The default value is 700 ( $\text{m}^{-1}\text{K}^{-1}$ ).		



Keyword	Definition			
	<b>Reactor Models</b>	<ul style="list-style-type: none"><li>• Diffusion or Premixed Opposed-flow Flame</li><li>• Burner-stabilized Pre-mixed Flame</li><li>• Premixed Laminar Flame-speed Calculation</li></ul>		
<b>EMSG</b>  Reactor Property Profiles	Approximation of the temperature-dependent emissivity of the gas-mixture, used to calculate a radiation-loss term in the gas energy equation. The radiation is calculated between the gas and the disk (using the gas temperature) and between the gas and the inlet (using the inlet temperature). The <b>EMSG</b> keyword provides temperature, emissivity pairs for the gas mixture.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Temperature</i>	Required	K	EMSG <b>20000.03</b>
	<i>Emissivity</i>	Required	--	EMSG 2000 <b>0.03</b>
	<b>Keyword Usage</b>	Optional keyword. By default, no gas radiation loss is included in the energy equation.		
	<b>Reactor Models</b>	<ul style="list-style-type: none"><li>• Rotating Disk CVD Reactor</li><li>• Stagnation Flow CVD Reactor</li></ul>		
<b>END</b>  Reactor Property	This keyword signifies the end of the input data for a given reactor description. It must appear after each set of data when continuation jobs are indicated using the <b>CNTN</b> keyword.			
	<b>Keyword Usage</b>	Required keyword.		
	<b>Reactor Models</b>	<ul style="list-style-type: none"><li>• Chemical and Phase Equilibrium Calculations</li><li>• Closed Homogeneous Batch Reactor</li><li>• Closed Partially Stirred Reactor (PaSR)</li><li>• Closed Plasma Reactor</li><li>• Cylindrical Shear Flow Reactor</li><li>• Diffusion or Premixed Opposed-flow Flame</li><li>• Honeycomb Reactor</li><li>• IC HCCI Engine</li><li>• Mechanism Analyzer</li><li>• Non-reactive Gas Mixer</li><li>• Normal Incident Shock</li><li>• Normal Reflected Shock</li><li>• Partially Stirred Reactor (PaSR)</li><li>• Perfectly Stirred Reactor (PSR)</li></ul>		

Keyword	Definition			
		<ul style="list-style-type: none"><li>Planar Shear Flow Reactor</li><li>Plasma Plug Flow Reactor</li><li>Plasma PSR</li><li>Plug Flow Reactor</li><li>Premixed Laminar Burner-stabilized Flame</li><li>Premixed Laminar Flame-speed Calculation</li><li>Rotating Disk CVD Reactor</li><li>SI Engine Zonal Simulator</li><li>Stagnation Flow CVD Reactor</li></ul>		
<b>EN-D-TIMEMAX</b>  Reactor Property	Since the physical time required to reach steady-state normally increases with decreasing values of SSDR, the integration time is increased by the factor SSDR_nominal/currentSSDR for SSDR values smaller than the nominal. The maximum value for the end-time is limited to the value specified by this control.			
	Parameters	Optional/Reqd.	Units	Examples
	Maximum value of end time	<b>Optional</b>	s	ENDTIMEMAX <b>1.0E+05</b>
	<b>Keyword Usage</b>	Optional keyword. The default value for the Diffusion Flamelet Generator is 1.0E+05		
	<b>Reactor Models</b>	<ul style="list-style-type: none"><li>Diffusion Flamelet Generator</li></ul>		
<b>ENGE</b>  Reactor Property	Solve the electron energy equation. The user must still specify a temperature (see <a href="#">ETMP</a> ), which provides the initial guess or initial value for the electron temperature.			
	Parameters	Optional/Reqd.	Units	Examples
	Reactor number (PSR clusters only)	Optional  If no number is given, values are assumed to apply to all reactors in a cluster.	--	ENGE <b>2</b>
	<b>Keyword Usage</b>	Optional keyword. By default, the electron energy equation is not solved.		
	<b>Reactor Models</b>	<ul style="list-style-type: none"><li>Closed Plasma Reactor</li></ul>		

Keyword	Definition			
		<ul style="list-style-type: none"><li>Plasma PSR</li><li>Plasma Plug Flow Reactor</li></ul>		
	Notes	<ul style="list-style-type: none"><li>ENGE must be specified when electrons are present for all PSRs.</li></ul>		
ENGY	Specifies the starting internal energy for the initial mixture.			
Reactor Property	Parameters	Optional/Reqd.	Units	Examples
	Energy	Required	erg/g	ENGY <b>1.5E9</b>
	Keyword Usage	Optional keyword. The user must specify two state variables and the composition to define the initial mixture.		
	Reactor Models	<ul style="list-style-type: none"><li>Chemical and Phase Equilibrium Calculations</li></ul>		
EN-RG	Solve the energy equation to determine the gas temperature.			
Problem Type	Parameters	Optional/Reqd.	Units	Examples
	Reactor number (PSR clusters only)	Optional  If no number is given, the keyword is assumed to apply to all reactors in a cluster.	--	ENRG <b>2</b>
	Keyword Usage	Optional keyword. Either TGIV or ENRG must be specified in most cases. For closed homogeneous systems, ICEN, CONP, CONV, or COTV can be specified instead. For Premixed Flamespeed Calculations, ENRG is required.		
	Reactor Models	<ul style="list-style-type: none"><li>Closed Homogeneous Batch Reactor</li><li>Closed Plasma Reactor</li><li>Diffusion or Premixed Opposed-flow Flame</li><li>Honeycomb Reactor</li><li>Non-reactive Gas Mixer</li><li>Perfectly Stirred Reactor (PSR)</li><li>Plasma Plug Flow Reactor</li></ul>		

Keyword	Definition			
		<ul style="list-style-type: none"><li>• Plasma PSR</li><li>• Plug Flow Reactor</li><li>• Premixed Laminar Flame-speed Calculation</li><li>• Premixed Laminar Burner-stabilized Flame</li><li>• Rotating Disk CVD Reactor</li><li>• Stagnation Flow CVD Reactor</li></ul>		
	Notes	<ul style="list-style-type: none"><li>• The user must still specify an initial or initial estimate of the gas temperature or temperature profile. See also: <a href="#">TEMP</a> or <a href="#">TPRO</a> keyword.</li><li>• For steady-state reactor models, this initial temperature is used in solving the intermediate fixed-temperature problem and is an initial guess for the solution of the full problem including the energy equation.</li><li>• Inclusion of the keywords <a href="#">CONP</a>, <a href="#">CONV</a>, or <a href="#">ICEN</a>, will also indicate that the energy equation should be solved.for closed homogeneous systems.</li></ul>		
ENTH	Specifies the starting enthalpy for the initial mixture.			
Reactor Property	Parameters	Optional/Reqd.	Units	Examples
	Enthalpy	Required	erg/g	ENTH <b>1.5E9</b>
	Keyword Usage	Optional keyword.The user must specify two state variables and the composition to define the initial mixture.		
	Reactor Models	<ul style="list-style-type: none"><li>• Chemical and Phase Equilibrium Calculations</li></ul>		
ENTH_DELTA_IN	Specifies the percentage with respect to the specified inlet enthalpy and is used to compute a new inlet temperature. For example, if the condition specified on the Inlet panel input is {T,Y_CH4}={300,1.0} and the input value for the enthalpy delta is -2%, then (a) the new enthalpy is $H_{new} = 0.98 * H(T=300, Y_{CH4}=1)$ , and (b) the new inlet temperature is $T_{new} = T(H_{new}, Y_{CH4})$ . The typical intended usage is to facilitate flamelet generation at different enthalpy levels. Note that when there is more than one inlet (as in the opposed-flow-based reactor models), the enthalpy change is applied to all inlets the same and, depending on the specified composition, each inlet will have a corresponding temperature.			
Reactor Property	Parameters	Optional/Reqd.	Units	Examples
	Percentage	Required	--	ENTH_DELTA_IN <b>5.0</b>
	Keyword Usage	Optional keyword.		
	Reactor Models	<ul style="list-style-type: none"><li>• Diffusion Flamelet Generator</li><li>• Extinction of Diffusion or Premixed Opposed-flow Flame</li></ul>		

Keyword	Definition			
		<ul style="list-style-type: none"><li>• Opposed-flow</li><li>• Premixed-Burner-Stabilized_Stagnation Flame</li></ul>		
EN-TR  Reactor Property	Specifies the starting entropy for the initial mixture.			
	Parameters	Optional/Reqd.	Units	Examples
	Entropy	Required	erg/(g · K)	ENTR <b>7.0E7</b>
	Keyword Usage	Optional keyword. The user must specify two state variables and the composition to define the initial mixture.		
	Reactor Models	<ul style="list-style-type: none"><li>• Chemical and Phase Equilibrium Calculations</li></ul>		
EPSG  Output	Threshold value for the first-order sensitivity coefficients for the growth rates of all bulk phases with respect to the rate constants. Coefficients below this value are neither printed to the diagnostic output file nor saved in the XML Solution File.			
	Parameters	Optional/Reqd.	Units	Examples
	Threshold value	Required	--	EPSG <b>.01</b>
	Keyword Usage	Optional keyword. By default, the threshold value for bulk phases is set to 0.001.		
	Reactor Models	<ul style="list-style-type: none"><li>• Closed Homogeneous Batch Reactor</li><li>• Closed Plasma Reactor</li><li>• Honeycomb Reactor</li><li>• Perfectly Stirred Reactor (PSR)</li><li>• Plasma Plug Flow Reactor</li><li>• Plasma PSR</li><li>• Plug Flow Reactor</li></ul>		
	Notes	<ul style="list-style-type: none"><li>• This keyword can be added but not removed from a continuation run.</li></ul>		
EPSR  Output	Threshold value for the rate-of-production coefficients. Coefficients below this value are neither printed to the diagnostic output file nor saved in the XML Solution File.			
	Parameters	Optional/Reqd.	Units	Examples
	Threshold value	Required	--	EPSR <b>.02</b>
	Keyword Usage	Optional keyword. By default, the threshold value for rate-of-production coefficients is set to 0.01.		
	Reactor Models	<ul style="list-style-type: none"><li>• Closed Homogeneous Batch Reactor</li><li>• Closed Plasma Reactor</li></ul>		

Keyword	Definition			
		<ul style="list-style-type: none"><li>• Honeycomb Reactor</li><li>• IC HCCI Engine</li><li>• Perfectly Stirred Reactor (PSR)</li><li>• Plasma Plug Flow Reactor</li><li>• Plasma PSR</li><li>• Plug Flow Reactor</li><li>• SI Engine Zonal Simulator</li></ul>		
	Notes	<ul style="list-style-type: none"><li>• This keyword can be added but not removed from a continuation run.</li></ul>		
EPSS  Output	Threshold value for the first-order sensitivity coefficients for the species with respect to the rate constants. Coefficients below this value are neither printed to the diagnostic output file nor saved in the XML Solution File.			
	Parameters	Optional/Reqd.	Units	Examples
	Threshold value	Required	--	EPSS <b>.01</b>
	Keyword Usage	Optional keyword. By default, the threshold value for species is set to 0.001.		
	Reactor Models	<ul style="list-style-type: none"><li>• Closed Homogeneous Batch Reactor</li><li>• Closed Plasma Reactor</li><li>• Diffusion or Premixed Opposed-flow Flame</li><li>• Honeycomb Reactor</li><li>• IC HCCI Engine</li><li>• Perfectly Stirred Reactor (PSR)</li><li>• Plasma Plug Flow Reactor</li><li>• Plasma PSR</li><li>• Plug Flow Reactor</li><li>• Premixed Laminar Burner-stabilized Flame</li><li>• Premixed Laminar Flame-speed Calculation</li><li>• Rotating Disk CVD Reactor</li><li>• SI Engine Zonal Simulator</li><li>• Stagnation Flow CVD Reactor</li></ul>		

Keyword	Definition			
	Notes	• This keyword can be added but not removed from a continuation run.		
EPST Output	Threshold value for the first-order sensitivity coefficients for the gas temperature with respect to the rate constants. Coefficients below this value are neither printed to the diagnostic output file nor saved in the XML Solution File.			
	Parameters	Optional/Reqd.	Units	Examples
	Threshold value	Required	--	EPST .01
	Keyword Usage	Optional keyword. By default, the threshold value for gas temperature is set to 0.001.		
	Reactor Models	• Closed Homogeneous Batch Reactor • Closed Plasma Reactor • Honeycomb Reactor • IC HCCI Engine • Perfectly Stirred Reactor (PSR) • Plasma Plug Flow Reactor • Plasma PSR • Plug Flow Reactor • SI Engine Zonal Simulator		
	Notes	• This keyword can be added but not removed from a continuation run.		
EQRX Solver	Specifies that the products from the premixed flame will be estimated by equilibrium calculation with constant enthalpy and pressure in the 2-zone SI Engine simulation. By default, equilibrium calculation is used to obtain gas product composition from the premixed flame.			
	Parameters	Optional/Reqd.	Units	Examples
	--	Optional	--	EQRX
	Keyword Usage	Optional keyword.		
	Reactor Models	• SI Engine Zonal Simulator		
EQUI Reactor Property	Flag indicating that equilibrium composition will be calculated. The chemical state of the statistical event particles will be determined by the corresponding equilibrium states instead of by time integration of the chemical source terms.			
	Keyword Usage	Optional keyword. By default, chemistry is neglected and a mixing-only calculation is performed. See also <a href="#">CHEM</a> .		
	Reactor Models	• Closed Partially Stirred Reactor (PaSR)		

Keyword	Definition			
		<ul style="list-style-type: none"><li>Partially Stirred Reactor (PaSR)</li><li>SI Engine Zonal Simulator</li></ul>		
EQUI  Reactor or Inlet Property	Specifies the air/fuel equivalence ratio for an inlet stream or for the initial conditions in a closed reactor.			
	Parameters	Optional/Reqd.	Units	Examples
	Inlet stream name (for open systems only)	Optional  If there is no stream name than the air/fuel equivalence ratio applies to the default or all defined streams.	--	EQUI <b>mixture1</b> 1.1
	Air / fuel equivalence ratio	Required	--	EQUI <b>1.1</b>
	Keyword Usage	Optional keyword. Either REAC or EQUI keywords are required for each inlet stream or to specify the initial conditions of a closed reactor. When EQUI is included, FUEL / OXID / CPROD keywords must also be supplied.		
	Reactor Models	<ul style="list-style-type: none"><li>Closed Homogeneous Batch Reactor</li><li>IC HCCI Engine</li><li>Perfectly Stirred Reactor (PSR)</li><li>Honeycomb Reactor</li><li>Plasma Plug Flow Reactor</li><li>Plasma PSR</li><li>Plug Flow Reactor</li></ul>		
ETCH  Reactor Property	Inclusion of this keyword indicates that a given bulk phase is expected to be etched instead of grown or deposited. This option changes the form of the equations to be solved for the bulk phase composition, as described in Bulk Species Equations During Etch of the Chemkin-Pro Theory Manual .			
	Parameters	Optional/Reqd.	Units	Examples
	Bulk phases	Optional	--	ETCH <b>BULK1</b>



Keyword	Definition			
		Required if there is more than one bulk phase		
	Reactor number (PSR clusters only)	Optional  If no number is given, the keyword is assumed to apply to all reactors in a cluster.	--	ETCH BULK1 2
	Keyword Usage	Optional keyword. By default, the names of the unnamed <i>Surface Kinetics</i> bulk phases is: BULK1, BULK2, etc.		
	Reactor Models	<ul style="list-style-type: none"><li>• Closed Homogeneous Batch Reactor</li><li>• Closed Plasma Reactor</li><li>• Honeycomb Reactor</li><li>• Perfectly Stirred Reactor (PSR)</li><li>• Plasma Plug Flow Reactor</li><li>• Plasma PSR</li><li>• Plug Flow Reactor</li><li>• Rotating Disk CVD Reactor</li><li>• Stagnation Flow CVD Reactor</li></ul>		
	Notes	<ul style="list-style-type: none"><li>• When the keyword <b>ETCH</b> is supplied for a bulk phase, it is required that bulk activities (see <b>BULK</b>) are also included for each bulk-phase species in that phase that is etched.</li></ul>		
ET-MP	The electron temperature in the reactor. This value is used as the initial estimate of the electron temperature for steady-state iteration (when <b>ENGE</b> is included), or as the initial electron temperature value for transient simulations.			
Reactor Property	Parameters	Optional/Reqd.	Units	Examples

Keyword	Definition			
	<i>Electron temperature</i>	Required	K	ETMP <b>33000.</b>
	<i>Reactor number (PSR clusters only)</i>	Optional  If no number is given, values are assumed to apply to all reactors in a cluster.	--	ETMP 33000. <b>1</b>
	<b>Keyword Usage</b>	Optional keyword. By default, the electron temperature is the same as the gas temperature.		
	<b>Reactor Models</b>	<ul style="list-style-type: none"><li>• Closed Plasma Reactor</li><li>• Plasma PSR</li><li>• Plasma Plug Flow Reactor</li></ul>		
<b>EXT_GET-FLAME-LETS</b>  Reactor Property	Compute extinguishing flamelets.			
	Parameters	Optional/Reqd.	Units	Examples
	--	Required when computing the extinguishing flamelets	--	EXT_GETFLAMELETS
	<b>Keyword Usage</b>	Optional.		
	<b>Reactor Models</b>	<ul style="list-style-type: none"><li>• Diffusion Flamelet Generator</li></ul>		
<b>EX-TINC-TION</b>  Reactor Property	Indicates extinction problem type.			
	<b>Keyword Usage</b>	Required keyword.		
	<b>Reactor Models</b>	<ul style="list-style-type: none"><li>• Extinction of Diffusion or Premixed Opposed-flow Flame</li></ul>		
<b>EXT_MAXTFRAC</b>  Reactor Property	The fraction multiplying the current T maximum that is used to constrain the flame toward extinction. The extinction simulator finds the location at which T = maximum temperature fraction * (Current maximum temperature — Inlet temperature). Temperature at this location is successively decreased by the user-specified temperature step size until it reaches T = minimum temperature fraction * (Current maximum temperature — Inlet temperature). A new location is then selected using the maximum temperature fraction. This process is repeated			

Keyword	Definition			
	until the desired number of steps is reached or until the flame is effectively extinguished.			
	Parameters	Optional/Reqd.	Units	Examples
	Maximum Temperature Fraction	Required	--	EXT_MAXTFRAC <b>0.8</b>
	Keyword Usage	Required. The default value is 10.8.		
	Reactor Models	• Extinction of Diffusion or Premixed Opposed-flow Flame		
	Notes	• Also see keyword <a href="#">EXT_MINTFRAC</a> .		
EXT_METHOD	Specifies the type of control technique to be used in extinction simulation.			
Reactor Property	Parameters	Optional/Reqd.	Units	Examples
	BOOLEAN	Required	--	EXT_METHOD <b>0</b>
	Keyword Usage	Optional. By default, the value is 0 which indicates 1-point control. The other possible choice is 1 which indicates 2-point control.		
	Reactor Models	• Extinction of Diffusion or Premixed Opposed-flow Flame		
EXT_MINTFLAME	If the maximum temperature in any solution obtained in the extinction simulation is below this value, the extinction simulator will stop assuming that there is no flame.			
Reactor Property	Parameters	Optional/Reqd.	Units	Examples
	Minimum Flame Temperature	Required	K	EXT_MINTFLAME <b>1500</b>
	Keyword Usage	Optional. The default value is 11500.		
	Reactor Models	• Extinction of Diffusion or Premixed Opposed-flow Flame		
	Notes	• This option is useful to avoid computing solutions beyond extinction point.		
EXT_MINTFRAC	The fraction multiplying the current T maximum that is used to constrain the flame toward extinction. The extinction simulator finds the location at which T = maximum temperature fraction * (Current maximum temperature — Inlet temperature). Temperature at this location is successively decreased by the user-specified temperature step size until it reaches T = minimum temperature fraction * (Current maximum temperature — Inlet temperature). A new location is then selected using the maximum temperature fraction. This process is repeated until the desired number of steps is reached or until the flame is effectively extinguished			
Reactor Property	Parameters	Optional/Reqd.	Units	Examples
	Minimum Temperature Fraction	Required	--	EXT_MINTFRAC <b>0.2</b>
	Keyword Usage	Required. The default value is 10.2.		

Keyword	Definition			
	Reactor Models	• Extinction of Diffusion or Premixed Opposed-flow Flame		
	Notes	• Also see keyword <a href="#">EXT_MAXTFRAC</a> .		
EXT_NIG- STEPS	Number of (internal) integration steps after which a flamelet file is written when computing extinguishing flamelets.			
Reactor Property	Parameters	Optional/Reqd.	Units	Examples
	<i>Number of integration steps</i>	Required when computing the extinguishing flamelets	--	EXT_NIGSTEPS <b>50</b>
	Keyword Usage	Optional. The default value is 50.		
	Reactor Models	• Diffusion Flamelet Generator		
EXT_SA- VEINT	Frequency of saving solution in extinction simulation.			
Reactor Property	Parameters	Optional/Reqd.	Units	Examples
	<i>Saving frequency</i>	Required	--	EXT_SAVEINT <b>10</b>
	Keyword Usage	Optional. The default value is 10.		
	Reactor Models	• Extinction of Diffusion or Premixed Opposed-flow Flame		
	Notes	• Since extinction problems are numerically intensive, it may be prudent to save solutions frequently. The input value of this keyword indicates the number of solutions are found before an opposed-flow solution is saved in the process of marching towards the extinction point. (A new extinction simulation can be started by using the restart facility.).		
EXT_STEPS	Number of times opposed flow solution is computed in search of the extinction point.			
Reactor Property	Parameters	Optional/Reqd.	Units	Examples
	<i>Solution steps</i>	Required	--	EXT_STEPS <b>100</b>
	Keyword Usage	Optional. The default value is 100.		
	Reactor Models	• Extinction of Diffusion or Premixed Opposed-flow Flame		
EXT_TSTEP	Temperature step by which temperature at control point is decreased in extinction simulator.			
Reactor Property	Parameters	Optional/Reqd.	Units	Examples
	<i>Temperature step</i>	Required	K	EXT_TSTEP <b>5</b>
	Keyword Usage	Optional. Default value is 5.		
	Reactor Models	• Extinction of Diffusion or Premixed Opposed-flow Flame		

Keyword	Definition			
<b>EXT_VFCNTRL</b>	Specifies how to constrain nozzle velocities in extinction simulation.			
Reactor Property	Parameters	Optional/Reqd.	Units	Examples
	<i>BOOLEAN</i>	Required	--	EXT_VFCNTRL <b>1</b>
	<b>Keyword Usage</b>	Required. The default value is 1 which indicates that momentum of the two jets should be balanced. This creates the stagnation plane in the middle. The other option is 0 which indicates that the magnitude of velocity from both nozzles is the same.		
	<b>Reactor Models</b>	<ul style="list-style-type: none"> <li>Extinction of Diffusion or Premixed Opposed-flow Flame</li> </ul>		
	<b>Notes</b>	<ul style="list-style-type: none"> <li>This option can only be used for 1-point control. For a 2-point control, it is ignored if specified.</li> </ul>		

## 10.2. Alphabetical Listing of Keywords [F-O]

Table 10.2: Alphabetical Listing of Keywords [F-O]

Keyword	Definition			
<b>FAZE</b>  Reactor Property	Specifies a fixed-phase constraint on the equilibrium calculation. Species that are initially in the gas phase will remain in the gas phase and species that are originally in a condensed phase (i.e., bulk species) will remain in that condensed phase. If there is only one phase in the chemistry set, the phase constraint has no effect.			
	<b>Keyword Usage</b>	Optional keyword. By default, phase equilibrium as well as composition equilibrium is determined.		
	<b>Reactor Models</b>	• Chemical and Phase Equilibrium Calculations		
<b>FGM_EXPORT</b>  Reactor Property	Write a Flamelet Generated Manifold file.			
	Parameters	Optional/Reqd.	Units	Examples
	--	Required when writing an FGM file	--	FGM_EXPORT
	<b>Keyword Usage</b>	Optional.		
	<b>Reactor Models</b>	• Diffusion Flamelet Generator		
<b>FICA0</b>  Inlet Property	The start of injection crank angle of the injection.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Injection name</i>	Required	--	FICA0 <b>main</b> -21.5
	<i>Crank angle</i>	Required	degree	FICA0 main <b>-21.5</b>
	<b>Keyword Usage</b>	Required keyword.		
<b>Reactor Models</b>	• Direct Injection Diesel Engine Simulator			

Keyword	Definition			
FIDUR  Inlet Property	Duration of injection in number of crank angles of the injection.			
	Parameters	Optional/Reqd.	Units	Examples
	Injection name	Required	--	FIDUR <b>main</b> 7.5
	Number of crank angle	Required	degree	FIDUR main <b>7.5</b>
	Keyword Usage	Required keyword.		
	Reactor Models	• Direct Injection Diesel Engine Simulator		
FILFY  Inlet Property	Initial liquid fuel component mass fraction of the injection			
	Parameters	Optional/Reqd.	Units	Examples
	Injection name	Required	--	FILFY <b>main</b> decalin 0.5
	Liquid component name	Required	--	FILFY main <b>decalin</b> 0.5
	Mass fraction	Required	--	FILFY main decalin <b>0.5</b>
	Keyword Usage	Required keyword.		
	Reactor Models	• Direct Injection Diesel Engine Simulator		
FIMAS  Inlet Property	Total liquid mass of the injection.			
	Parameters	Optional/Reqd.	Units	Examples
	Injection name	Required	--	FIMAS <b>main</b> 0.055
	Total injection mass	Required	g	FIMAS main <b>0.055</b>
	Keyword Usage	Required keyword.		
	Reactor Models	• Direct Injection Diesel Engine Simulator		
FINJP  Inlet Property	A piecewise-linear continuous profile can be used to describe a non-uniform injection rate profile. The piecewise profile should be given by a series of data points of normalized crank angle and injection rate pair. The normalized crank angle (CA) data must be arranged in ascending order from 0.0 to 1.0. The injection rate data are in arbitrary units and the direct injection (DI) engine model will rescale the injection rate data to match the total injection mass. By default, a uniform injection rate profile based on the total injection mass and the duration of injection is assumed.			
	Parameters	Optional/Reqd.	Units	Examples
	Injection name	Required	--	FINJP <b>injection1</b> 0.5 0.75
	Crank angle	Required	--	FINJP injection1 <b>0.5</b> 0.75
	Injection rate	Required	--	FINJP injection1 0.5 <b>0.75</b>
	Keyword Usage	Optional keyword.		
	Reactor Models	• Direct Injection Diesel Engine Simulator		
	FINRD	Number of divisions (rings) in the radial direction to be applied to the injection. The injection/spray is divided into parcels. The total number of parcels is		

Keyword	Definition			
Inlet Property	determined by multiplying the number of divisions in the radial direction by the number of divisions in the time/injection direction.			
	Parameters	Optional/Reqd.	Units	Examples
	Injection name	Required	--	FINRD <b>main</b> 10
	Number of divisions	Required	--	FINRD main <b>10</b>
	Keyword Usage	Required keyword.		
	Reactor Models	• Direct Injection Diesel Engine Simulator		
FINTL Inlet Property	Number of divisions in the time/injection direction to be applied to the injection. The injection/spray is divided into parcels. The total number of parcels is determined by multiplying the number of divisions in the radial direction by the number of divisions in the time/injection direction.			
	Parameters	Optional/Reqd.	Units	Examples
	Injection name	Required	--	FINTL <b>main</b> 10
	Number of divisions	Required	--	FINTL main <b>10</b>
	Keyword Usage	Required keyword.		
	Reactor Models	• Direct Injection Diesel Engine Simulator		
FIT-MP Inlet Property	Initial liquid temperature of the injection.			
	Parameters	Optional/Reqd.	Units	Examples
	Injection name	Required	--	FITMP <b>main</b> 345.5
	Liquid temperature	Required	K	FITMP main <b>345.5</b>
	Keyword Usage	Required keyword.		
	Reactor Models	• Direct Injection Diesel Engine Simulator		
FIXT Reactor Property	Specifies a fixed-temperature boundary condition on the upper wall (only used for non-symmetric cartesian coordinates).			
	Parameters	Optional/Reqd.	Units	Examples
	Temperature	Optional, if a temperature is not specified, the value of the inlet gas temperature will be used (TINL)	K	FIXT <b>400</b>
	Keyword Usage	Optional keyword. By default, a zero temperature gradient is enforced if FIXT is omitted (adiabatic upper wall)		
	Reactor Models	• Planar Shear Flow Reactor		

Keyword	Definition			
FLAM  Reactor Property	Position and fixed-temperature value for calculating strained, lifted flames. In this case, the inlet gas velocity is calculated (rather than fixed) based on a fixed location of the flame front. The flame front location is specified by giving a location and value of a temperature (above the inlet temperature value) to fix at this position.			
	Parameters	Optional/Reqd.	Units	Examples
	Flame position	Required	cm	FLAM <b>0.5700</b> .
	Temperature	Required	K	FLAM 0.5 <b>700</b> .
	Keyword Usage	Optional keyword. By default, no temperature is fixed in the calculation.		
	Reactor Models	<ul style="list-style-type: none"><li>Rotating Disk CVD Reactor</li><li>Stagnation Flow CVD Reactor</li></ul>		
FLINJ  Inlet Property	Assign an injection to an injector.			
	Parameters	Optional/Reqd.	Units	Examples
	Injection name	Required	--	FLINJ <b>modelX</b> pilot1
	Injector name	Required	--	FLINJ  modelX <b>pilot1</b>
	Keyword Usage	Required keyword.		
	Reactor Models	<ul style="list-style-type: none"><li>Direct Injection Diesel Engine Simulator</li></ul>		
FLRT  Inlet Property	The mass flow rate into the reactor for an optionally specified inlet stream. For Premixed Laminar Flame calculations, this is mass flux at the inlet (mass flow rate per area) and there is no option for inlet stream name.			
	Parameters	Optional/Reqd.	Units	Examples
	Inlet stream name (Not valid for Premixed Laminar Flames)	Optional  If there is no stream name then the mass flow rate applies to the default or to all defined streams.	--	FLRT <b>secondary_air</b> 0.13
	Mass flow rate or Mass flux (for Premixed Laminar Flames)	Required	g/sec  g/(cm <sup>2</sup> · sec)	FLRT secondary_air <b>0.13</b>  FLRT 0.04



Keyword	Definition			
	Keyword Usage	<b>PFRs and Monolith Reactors:</b> Flow specification via one of <a href="#">VEL</a> , <a href="#">VDOT</a> , <a href="#">VDOTPRO</a> , <a href="#">SCCM</a> , <a href="#">SCCMPRO</a> , <a href="#">FLRT</a> , or <a href="#">FPRO</a> is required. PSRs and PaSRs: Optional keyword. If none of <a href="#">TAU</a> , <a href="#">FLRT/FPRO</a> , <a href="#">SCCM/SCCMPRO</a> are specified or are nonzero, then a closed-system is assumed. <a href="#">FLRT/FPRO</a> or <a href="#">SCCM/SCCMPRO</a> is required for each <a href="#">INLET</a> stream defined. Premixed Laminar Flames: Required keyword. Stagnation Flow CVD Reactors: <a href="#">FLRT</a> / <a href="#">FPRO</a> or <a href="#">SCCM</a> / <a href="#">SCCMPRO</a> or <a href="#">UINL</a> is required for each inlet stream defined. Rotating Disk CVD Reactors: Optional keyword.		
	Reactor Models	<ul style="list-style-type: none"><li>• Honeycomb Monolith Reactor</li><li>• Non-reactive Gas Mixer</li><li>• Partially Stirred Reactor (PaSR)</li><li>• Perfectly Stirred Reactor (PSR)</li><li>• Plasma PFR</li><li>• Plasma PSR</li><li>• Plug Flow Reactor</li><li>• Premixed Laminar Burner-stabilized Flame</li><li>• Premixed Laminar Flame-speed Calculation</li><li>• Rotating Disk CVD Reactor</li><li>• Stagnation Flow CVD Reactor</li></ul>		
<b>FLTB_FGM</b>	Specifies the name of the Flamelet Generation Manifold (FGM) file.			
Reactor Property	Parameters	Optional/Reqd.	Units	Examples
	FGM file name	Required when writing an FGM file	--	FLTB_FGM <b>Diffusion_FGM fla</b>
	Keyword Usage	Optional.		
	Reactor Models	<ul style="list-style-type: none"><li>• Diffusion Flamelet Generator</li></ul>		
<b>FLT_NPOINTS</b>	Specifies number of grid points in the progress-variable space.			
Reactor Property	Parameters	Optional/Reqd.	Units	Examples
	Number of progress variable points	Required when writing FGM file	--	FLT_NPOINTS <b>50</b>

Keyword	Definition			
	<b>Keyword Usage</b>	Optional. The default value is 50.		
	<b>Reactor Models</b>	• Diffusion or Premixed Opposed-flow Flame		
<b>FLT_PVSPEC</b>	Species name and its mass-fraction weighting factor to be used in the calculation of the rate-of-progress variable when generating flamelet tables (for premixed flames).			
Reactor Property	Parameters	Optional/Reqd.	Units	Examples
	<i>Species name</i>	Required	--	FLT_PVSPEC <b>CO2</b> 1.2
	<i>Mass-fraction weighting factor</i>	Required	--	FLT_PVSPEC CO2 <b>1.2</b>
	<b>Keyword Usage</b>	Required keyword when generating flamelet table.		
	<b>Reactor Models</b>	• Rotating Disk CVD Reactor  • Stagnation Flow CVD Reactor		
<b>FLTB</b>	Export one-dimensional flamelet tables in the standard flamelet format to the specified file. The file will be created in the working directory.			
Output	Parameters	Optional/Reqd.	Units	Examples
	<i>Flamelet table filename</i>	Required	--	FLTB <b>flamelet.txt</b>
	<b>Keyword Usage</b>	Optional keyword. By default, no flamelet table is exported. The name of the flamelet table file generated is FileName_1.FileExt (where FileName is the user-provided name; FileName= flamelet and FileExt=txt in the example given here.) When continuations are used, the filename is appended with “_n” where n is the continuation number+1 . For extinction studies, the flamelet files are generated based on <i>input “Step Interval for Saving (EXT_SAVEINT)”</i> . Thus, “_n” in the flamelet filename generated in the extinction study indicates the ( <i>total steps/EXT_SAVEINT</i> ).		
	<b>Reactor Models</b>	• - Opposed-flow Flame Simulator		
<b>FLUX</b>	This keyword indicates that a flux balance will determine the mass fractions of the species at the inlet (rather than a fixed composition). If <b>FLUX</b> is specified, the <b>REAC</b> keywords are used to determine the convective mass flux in, which is balanced against diffusive fluxes to dynamically determine the inlet gas composition. See <a href="#">Equation 14.21</a> of the <a href="#">Chemkin-Pro Theory Manual</a> .			
Reactor Property	<b>Keyword Usage</b>	Optional keyword. By default, a flux balance is solved at the inlet. See also <a href="#">COMP</a> .		
	<b>Reactor Models</b>	• Rotating Disk CVD Reactor  • Stagnation Flow CVD Reactor		
<b>FLXB</b>	Use extrapolation to obtain species mass fractions at the outflow (or hot) boundary. By default, PREMIX assumes all species have zero mass fraction			

Keyword	Definition			
Reactor Property	gradients at the outflow boundary. However, for pollutant species such as NO, their concentrations are still growing in the post flame region so that their mass fraction profiles have positive gradients at the outflow boundary. The extrapolation boundary condition provides a proper outflow treatment when mass fraction gradients are not zero at the outflow boundary.			
	Keyword Usage	Optional keyword. By default, zero mass fraction gradient is used as outflow boundary condition		
	Reactor Models	<ul style="list-style-type: none"><li>• Premixed Laminar Burner-stabilized Flame</li><li>• Premixed Laminar Flame-speed Calculation</li></ul>		
FPRO  Inlet Property Profiles	Used to specify a transient profile or function of mass flow rate vs. time for an inlet stream. The profile specified will be interpolated linearly from the <a href="#">FPRO</a> points provided.			
	Parameters	Optional/Reqd.	Units	Examples
	Inlet stream name	Optional  If there is no stream name then the reactant and mole fraction apply to all streams.	--	FPRO <b>purge</b> 0.19 29.0
	Time	Required	sec (cm for flow reactors)	FPRO <b>0.19</b> 29.0
	Flow rate	Required	g/sec	FPRO 0.19 <b>29.0</b>
	Keyword Usage	<b>PFRs and Monolith Reactors:</b> Flow specification via one of <a href="#">VEL</a> , <a href="#">VDOT</a> , <a href="#">VDOTPRO</a> <a href="#">SCCM</a> <a href="#">SCCMPRO</a> <a href="#">FLRT</a> , or <a href="#">FPRO</a> is required. PSRs and PaSRs: Optional keyword. If none of <a href="#">TAU</a> , <a href="#">FLRT</a> / <a href="#">FPRO</a> , <a href="#">SCCM</a> / <a href="#">SCCMPRO</a> are specified or are nonzero, then a closed-system is assumed. <a href="#">FLRT</a> / <a href="#">FPRO</a> or <a href="#">SCCM</a> / <a href="#">SCCMPRO</a> is required for each <a href="#">INLET</a> stream defined. Premixed Laminar Flames: Required keyword. Stagnation Flow CVD Reactors: <a href="#">FLRT</a> / <a href="#">FPRO</a> or <a href="#">SCCM</a> / <a href="#">SCCMPRO</a> or <a href="#">UINL</a> is required for each inlet stream defined. Rotating Disk CVD Reactors: Optional keyword.		
	Reactor Models	<ul style="list-style-type: none"><li>• Honeycomb Monolith Reactor.</li><li>• Non-reactive Gas Mixer</li></ul>		

Keyword	Definition			
		<ul style="list-style-type: none"><li>• Perfectly Stirred Reactor (PSR)</li><li>• Plasma PFR</li><li>• Plasma PSR</li><li>• Plug Flow Reactor (PFR)</li><li>• Rotating Disk CVD Reactor</li><li>• Stagnation Flow CVD Reactor</li></ul>		
FREE  Reactor Property	Specifies that the equilibrium species composition will be calculated. See also <a href="#">FROZ</a> .			
	Keyword Usage	Optional keyword. By default, the composition will be calculated.		
	Reactor Models	<ul style="list-style-type: none"><li>• Chemical and Phase Equilibrium Calculations</li></ul>		
FREE  Reactor Property	Specifies the problem type, which will be to solve for a freely propagating flame to determine flame speed.			
	Keyword Usage	Required keyword.		
	Reactor Models	<ul style="list-style-type: none"><li>• Premixed Laminar Flame-speed Calculation</li></ul>		
	Notes	<ul style="list-style-type: none"><li>• The problem-type can be changed for a restart run. See also <a href="#">BURN</a>.</li></ul>		
FROZ  Reactor Property	Specifies that species composition will be frozen or fixed during the equilibrium calculation. See also <a href="#">FREE</a> .			
	Keyword Usage	Optional keyword. By default, the composition will be calculated.		
	Reactor Models	<ul style="list-style-type: none"><li>• Chemical and Phase Equilibrium Calculations</li></ul>		
FUEL  Inlet or Reactor Property	Defines the fuel mole fraction composition for an inlet stream in an open system or for the initial conditions in a closed system, when an equivalence ratio is specified ( <a href="#">EQUI</a> ). It must be followed by a species name and then the mole fraction. One of these <a href="#">FUEL</a> inputs must appear for each fuel species, which are used to determine the inlet composition based on an equivalence-ratio calculation. Any given species can participate simultaneously as a fuel, oxidizer, or product. The sum of all the fuel mole fractions should equal one. If it does not, a warning message will be printed and the mole fractions will be normalized so the sum does equal one.			
	Parameters	Optional/Reqd.	Units	Examples
	Inlet stream name (PSRs only)	Optional  If there is no stream name	--	FUEL <b>mixture1</b> C2H2 0.5

Keyword	Definition			
		than the fuel mole fraction compassion applies to the default or all defined streams.		
	Species name	Required	--	FUEL <b>C2H20.5</b>
	Fuel fraction	Required	mole fractions	FUEL C2H2 <b>0.5</b>
	Keyword Usage	Required keyword when <a href="#">EQUI</a> option is used for an inlet stream or for the initial conditions in a reactor.		
	Reactor Models	<ul style="list-style-type: none"><li>• Closed Homogeneous Batch Reactor</li><li>• Honeycomb Reactor</li><li>• IC HCCI Engine</li><li>• Perfectly Stirred Reactor</li><li>• Plasma Plug Flow Reactor</li><li>• Plasma PSR</li><li>• Plug Flow Reactor</li><li>• SI Engine Zonal Simulator</li></ul>		
	Notes	<ul style="list-style-type: none"><li>• The mole fractions are of the fuel itself, not for the entire composition.</li><li>• The <a href="#">FUEL</a> keywords must be changed as a set, not individually for a restart run.</li><li>• The <a href="#">FUEL</a> keywords must be changed as a set, not individually for continuation run.</li></ul>		
	FVCP	Specify the piecewise linear profile of the friction velocity coefficient when the wall-function heat transfer correlation is used to compute wall heat loss rate. Note that Chemkin-Pro requires the friction velocity to be given in cm/sec. Although the friction velocity coefficient <b>f</b> should be dimensionless, users should scale its value to convert the units of the friction velocity to cm/sec. For more information about this heat transfer correlation, see the <a href="#">Chemkin-Pro Theory Manual</a> .		
Reactor Property	Parameters	Optional/Reqd.	Units	Examples
	Crank angle	Required	degree	FVCP - <b>120.2</b> 10.0
	Friction velocity coefficient	Required	--	FVCP -120.2 <b>10.0</b>

Keyword	Definition			
	Keyword Usage	Optional keyword.		
	Reactor Models	<ul style="list-style-type: none"><li>Multi-Zone HCCI Simulator</li><li>IC HCCI Engine</li><li>SI Engine Zonal Simulator</li></ul>		
GASW	Estimated gas-phase mole fractions at the wall boundaries, which may be helpful to aid in convergence. The sum of all the GASW values should equal one. However, if they do not, a cautionary message will be printed and the mole fractions will be normalized so the sum does equal one. The actual gas mole fractions at each wall at the initial condition of the boundary-layer calculation will be calculated via the Twopnt procedure (unless the NOTP keyword appears).			
Reactor Property	Parameters	Optional/Reqd.	Units	Examples
	Gas species name	Required	--	GASW SIH21.0E-4
	Mole fraction of gas species	Required	mole fractions	GASW SIH2 1.0E-4
	Keyword Usage	Optional keyword. By default, values given by the REAC keyword will be used.		
	Reactor Models	<ul style="list-style-type: none"><li>Cylindrical Shear Flow Reactor</li><li>Planar Shear Flow Reactor</li></ul>		
GDOT	This keyword may be used to specify explicitly the net surface production rates of gas-phase species at the substrate, instead of using Surface Kinetics. In order to use this option, the Surface Kinetics input file must be empty, which means that the number of surface reactions, surface site species and bulk species must all be zero in the Surface Kinetics input file.			
Reactor Property	Parameters	Optional/Reqd.	Units	Examples
	Species name	Required	--	GDOT H -1.3E-7
	Net surface production rate	Required	mole/cm <sup>2</sup> sec	GDOT H -1.3E-7
	Keyword Usage	Optional keyword. By default, the net surface production rate is 0.0.		
	Reactor Models	<ul style="list-style-type: none"><li>Rotating Disk CVD Reactor</li><li>Stagnation Flow CVD Reactor</li></ul>		
GEN	Controls the printing of general information about the chemistry set. It also controls the printing of summary tables about the reaction thermodynamics. The ALL option produces all of the general information tables. NONE will suppress this output. If only GEN is given on the input line, ALL is assumed (the default). The GEN information is printed by default unless explicitly turned off.			
Output	Parameters	Optional/Reqd.	Units	Examples
	ALL option	Optional	--	GEN ALL
	NONE option	Optional	--	GEN NONE

Keyword	Definition			
	<b>Keyword Usage</b>	Optional keyword. By default, the table output is determined by the <a href="#">ALL</a> or <a href="#">NONE</a> keyword.		
	<b>Reactor Models</b>	<ul style="list-style-type: none"><li>Mechanism Analyzer</li></ul>		
<b>GFAC</b>  Reactor Property	This keyword specifies that the rates of all gas-phase reactions will be multiplied (scaled) by the factor <a href="#">GFAC</a> . This option is sometimes useful if convergence difficulties are encountered due to unusually large reaction rates. Using <a href="#">GFAC</a> , the problem can first be first solved with artificially reduced reaction rates, which then can be increased in subsequent continuations or restarts until <a href="#">GFAC</a> is one. In addition, setting <a href="#">GFAC</a> and <a href="#">SFAC</a> to zero for a perfectly stirred reactor simulation, enables the Non-reactive Gas Mixer Reactor Model.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Multiplier value</i>	Required	--	GFAC <b>2.0</b>
	<i>Reactor number (PSR clusters only)</i>	Optional  If no number is given, values are assumed to apply to all reactors in a cluster.	--	GFAC 2.0 <b>1</b>
	<b>Keyword Usage</b>	<b>General:</b> Optional keyword. By default, the multiplier value is set to 1.0.  Non-reactive Mixer: Required keyword, must be set to 0.0 to enable this Reactor Model.		
<b>Reactor Models</b>	<ul style="list-style-type: none"><li>Closed Homogeneous Batch Reactor</li><li>Closed Plasma Reactor</li><li>Cylindrical Shear Flow Reactor</li><li>Diffusion or Premixed Opposed-flow Flame</li><li>Honeycomb Reactor</li><li>IC HCCI Engine</li><li>Non-reactive Gas Mixer</li><li>Perfectly Stirred Reactor (PSR)</li><li>Planar Shear Flow Reactor</li><li>Plasma Plug Flow Reactor</li></ul>			

Keyword	Definition			
		<ul style="list-style-type: none"><li>• Plasma PSR</li><li>• Plug Flow Reactor</li><li>• Premixed Laminar Burner-stabilized Flame</li><li>• Premixed Laminar Flame-speed Calculation</li><li>• Rotating Disk CVD Reactor</li><li>• SI Engine Zonal Simulator</li><li>• Stagnation Flow CVD Reactor</li></ul>		
GMHTC  Reactor Property	The reactor wall temperature will be obtained by solving energy conservation equation for the reactor wall. It uses the heat transfer coefficient between the inner wall surface and the gas mixture inside the reactor specified by GMHTC. The initial wall temperature is the surface temperature. When this option is used, all the external heat fluxes, i.e., heat loss to the environment and heat exchange between the reactors in a network, are applied to the wall energy equation instead of the gas phase energy equation. The heat generated by the surface reactions will also be included in the wall energy equation.			
	Parameters	Optional/Reqd.	Units	Examples
	Material name	<b>Optional.</b>  If no material is specified, the same value will be used for all materials.	--	GMHTC <b>material10.1</b>
	Heat transfer coefficient	Required	cal/(cm <sup>2</sup> -K-sec)	GMHTC <b>0.1</b>
	Reactor number (PSR clusters only)	<b>Optional.</b>  If no number is given, the keyword is assumed to apply to all reactors	--	GMHTC material1 0.1 <b>1</b>



Keyword	Definition			
		in a cluster.		
	Keyword Usage	Optional keyword. This keyword must be used with <a href="#">MMASS</a> . By default, the wall energy equation will not be solved and the reactor wall temperature is equal to the gas temperature in the reactor unless the surface temperature is specified.		
	Reactor Models	<ul style="list-style-type: none"><li>• Closed Homogeneous Batch Reactor</li><li>• Closed Plasma Reactor</li><li>• Honeycomb Monolith Reactor</li><li>• IC HCCI Engine</li><li>• Non-reactive Gas Mixer</li><li>• Perfectly Stirred Reactor (PSR)</li><li>• Plasma PSR</li><li>• Plasma Plug Flow Reactor</li><li>• Plug Flow Reactor</li><li>• SI Engine Zonal Simulator</li></ul>		
GRAD  Reactor Property	Parameter that controls the degree of mesh adaptation based on the maximum first derivative, or gradient in the solution. A reasonable value is usually between about 0.1 and 1.0, where no adaptation based on gradient is specified with 1.0.			
	Parameters	Optional/Reqd.	Units	Examples
	Gradient of mesh adaptation	Required	--	GRAD <b>0.5</b>
	Keyword Usage	Optional keyword. By default, the gradient is set to 0.1.		
	Reactor Models	<ul style="list-style-type: none"><li>• Diffusion or Premixed Opposed-flow Flame</li><li>• Premixed Laminar Burner-stabilized Flame</li><li>• Premixed Laminar Flame-speed Calculation</li><li>• Rotating Disk CVD Reactor</li><li>• Stagnation Flow CVD Reactor</li></ul>		
	Notes	<ul style="list-style-type: none"><li>• This keyword can be changed for a restart or continuation run.</li><li>• <a href="#">Steady-state 1-D Solution Methods</a> of the <a href="#">Chemkin-Pro Theory Manual</a> for more information.</li></ul>		

Keyword	Definition			
GRAV  Reactor Property	The value of the acceleration of gravity. The buoyancy term can only be included in the boundary-layer equations if gravity acts parallel to the principal flow direction. Thus, GRAV 980 may be used to describe flow vertically upward, or GRAV -980 for flow downward. Omitting this keyword neglects the buoyancy term.			
	Parameters	Optional/Reqd.	Units	Examples
	Acceleration of gravity	Required	cm/sec <sup>2</sup>	GRAV <b>-980</b>
	Keyword Usage	Optional keyword. By default, the acceleration of gravity is zero.		
	Reactor Models	<ul style="list-style-type: none"><li>• Cylindrical Shear Flow Reactor</li><li>• Planar Shear Flow Reactor</li></ul>		
GRID  Reactor Property Profiles	Specifies a point on an initial grid. Up to <b>NTOT</b> of these <b>GRID</b> inputs can be included. Each <b>GRID</b> entry contains the spatial coordinate of a mesh point. The <b>GRID</b> keywords are a grouped list and the grid coordinates must appear in ascending order.			
	Parameters	Optional/Reqd.	Units	Examples
	mesh point coordinate	Required	cm	GRID <b>0.0</b>
	Keyword Usage	Optional keyword. If no <b>GRID</b> keywords are included, the grid will have equally spaced grid points based on the value of <b>NPTS</b> .		
	Reactor Models	<ul style="list-style-type: none"><li>• Diffusion or Premixed Opposed-flow Flame</li><li>• Premixed Laminar Burner-stabilized Flame</li><li>• Premixed Laminar Flame-speed Calculation</li><li>• Rotating Disk CVD Reactor</li><li>• Stagnation Flow CVD Reactor</li></ul>		
GRXN  Output	Prints out a table of reaction rates and other pertinent information for each gas-phase reaction. The <b>ALL</b> option is the default and produces tables for every gas-phase reaction. The <b>NONE</b> option suppresses output for all of the reactions. If reaction information is desired for only certain reactions, they may be optionally specified by their number (given in the Pre-processor output) or by typing an exact duplicate of the reaction expression (see example input).			
	Parameters	Optional/Reqd.	Units	Examples
	ALL option	Optional, default is ALL	--	GRXN <b>ALL</b>
	NONE option	Optional, de-	--	GRXN <b>NONE</b>

Keyword	Definition			
		<b>fault is ALL</b>		
	<i>Gas reaction number list</i>	<b>Optional, default is ALL</b>	--	GRXN <b>2 5</b>
	<i>Gas reaction expression</i>	<b>Optional, default is ALL</b>	--	GRXN <b>CH4+H&lt;=&gt;CH3+H2</b>
	<b>Keyword Usage</b>	Optional keyword. By default, the table output is determined by the <a href="#">ALL</a> or <a href="#">NONE</a> keyword.		
	<b>Reactor Models</b>	• Mechanism Analyzer		
<b>GTHB</b> Output	Create an extra table of the reaction rates for those reactions that involve third bodies. This option employs the bath-gas composition (specified by the <a href="#">XBTH</a> keyword) to yield effective reaction rates. The <a href="#">ALL</a> option is the default and produces tables for every gas-phase reaction. The <a href="#">NONE</a> option suppresses output for all of the reactions. If reaction information is desired for only certain reactions, they may be optionally specified by their number (given in the Pre-processor output) or by typing an exact duplicate of the reaction expression (see example input).			
	Parameters	Optional/Reqd.	Units	Examples
	<i>ALL option</i>	<b>Optional, default is ALL</b>	--	GTHB <b>ALL</b>
	<i>NONE option</i>	<b>Optional, default is ALL</b>	--	GTHB <b>NONE</b>
	<i>Gas reaction number list</i>	<b>Optional, default is ALL</b>	--	GTHB <b>2 5</b>
	<i>Gas reaction expression</i>	<b>Optional, default is ALL</b>	--	GTHB <b>2H+M&lt;=&gt;H2+M</b>
	<b>Keyword Usage</b>	Optional keyword. By default, the table output is determined by the <a href="#">ALL</a> or <a href="#">NONE</a> keyword.		
	<b>Reactor Models</b>	• Mechanism Analyzer		
<b>GVEL</b> Reactor Property	Activate the Woschni correlation for the average cylinder gas velocity. This keyword can only be used in conjunction with the <a href="#">ICHT</a> keyword. <a href="#">Internal Combustion Engine Model</a> of the <a href="#">Chemkin-Pro Theory Manual</a> .			
	Parameters	Optional/Reqd.	Units	Examples

Keyword	Definition			
	$C_{11}$ in the average gas velocity correlation	Required	--	GVEL <b>2.28</b> 0.308 0.324 0
	$C_{12}$ parameter in the Woschni correlation	Required	cm/(sec · K)	GVEL 2.28 <b>0.308</b> 0.324 0
	$C_2$ parameter in the Woschni correlation	Required		GVEL 2.28 0.308 <b>0.324</b> 0
	Ratio of swirl velocity to mean piston speed	Required	--	GVEL 2.28 0.308 0.324 <b>0</b>
	<b>Keyword Usage</b>	Optional keyword. By default, the setting is GVEL 1 0 0 0.		
	<b>Reactor Models</b>	<ul style="list-style-type: none"><li>• IC HCCI Engine</li><li>• SI Engine Zonal Simulator</li></ul>		
<b>HIMP</b> Reactor Property	Use the Huber correlation to calculate the characteristic gas velocity used by the Woschni heat transfer coefficient formulation.			
	Parameters	Optional/Reqd.	Units	Examples
	IMEP	Required	atm	HIMP <b>10</b>
	<b>Keyword Usage</b>	This keyword is optional and works when the Woschni heat transfer formulations (ICHT, ICHX, and ICHW) and the Woschni gas velocity correlation (GVEL) are also in use.		
	<b>Reactor Models</b>	<ul style="list-style-type: none"><li>• IC HCCI Engine</li><li>• Multi-Zone HCCI Engine</li><li>• SI Engine Zonal Simulator</li></ul>		
<b>HITE</b> Reactor Property	The channel height (for cartesian coordinates), or the reactor radius ( cylindrical coordinates), or distance between the channel wall and the symmetry line for a symmetric planar channel.			
	Parameters	Optional/Reqd.	Units	Examples
	Channel height or radius	Required	cm	HITE <b>2.0</b>
	<b>Keyword Usage</b>	Required keyword.		
	<b>Reactor Models</b>	<ul style="list-style-type: none"><li>• Cylindrical Shear Flow Reactor</li><li>• Planar Shear Flow Reactor</li></ul>		
<b>H0</b> Solver	The initial distance step size used by the transient solver.			
	Parameters	Optional/Reqd.	Units	Examples
	Initial time step size	Required	cm	H0 <b>1.0E-4</b>

Keyword	Definition			
	Keyword Usage	Optional keyword. By default, the initial time step size is set to 1.0E-6.		
	Reactor Models	<ul style="list-style-type: none"><li>Cylindrical Shear Flow Reactor</li><li>Planar Shear Flow Reactor</li></ul>		
HP	Constant pressure and enthalpy constraints.			
Problem Type	Keyword Usage	Optional keyword. Exactly one problem type keyword must be included.		
	Reactor Models	<ul style="list-style-type: none"><li>Chemical and Phase Equilibrium Calculations</li></ul>		
	Notes	<ul style="list-style-type: none"><li>PH keyword is equivalent.</li></ul>		
HSEN	Calculate the first-order, heat-of-formation sensitivity coefficients (i.e., with respect to the gas-phase and surface species heats of formation) for species fractions and for other dependent variables in the system. Sensitivity results will be included in the XML Solution File.			
Output	Parameters	Optional/Reqd.	Units	Examples
	String indicating for which variables sensitivity coefficients will be saved or printed. The string is a space-delimited list containing species names and any one of the following: ALL, AVEL, RVEL, CVEL, FLRT, or TEMP (see Notes)	Optional  If no string is given, then ALL is assumed.	--	HSEN OH  HSEN TEMP
	Keyword Usage	Optional keyword. By default, no sensitivity coefficients are computed or printed.		
	Reactor Models	<ul style="list-style-type: none"><li>Diffusion or Premixed Opposed-flow Flame</li><li>Premixed Laminar Burner-stabilized Flame</li><li>Premixed Laminar Flame-speed Calculation</li><li>Rotating Disk CVD Reactor</li><li>Stagnation Flow CVD Reactor</li></ul>		
	Notes	<ul style="list-style-type: none"><li>This keyword can be added but not removed from a continuation or restart run</li><li>See also EPSS, EPSG, EPST, SENG, and HSEN for other sensitivity options</li></ul>		

Keyword	Definition			
		The optional parameter strings are defined as follows: <ul style="list-style-type: none"><li>• ALL: all species and all other dependent variables in the solution</li><li>• AVEL: axial velocity (Plug Flow, Diffusion or Premixed Opposed-flow Flames, Rotating Disk, and Stagnation Flow CVD Reactors only)</li><li>• CVEL: circumferential velocity (Rotating Disk and Stagnation Flow CVD Reactors only)</li><li>• RVEL: radial velocity (Diffusion or Premixed Opposed-flow Flames, Rotating Disk, and Stagnation Flow CVD Reactors only)</li><li>• FLRT: mass flow rate (Premixed Laminar Flame-speed Calculation only)</li><li>• TEMP: gas temperature</li></ul>		
HSWC Reactor Property	Specifies the crank angle when the entire wall heat loss will be switched from the unburned zone to the burned zone. <a href="#">HSWM</a> , <a href="#">HSWT</a> , and <a href="#">HSWC</a> are mutually exclusive.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Crank angle</i>	Required	degree	HSWC <b>-0.4</b>
	Keyword Usage	Optional keyword.		
	Reactor Models	• SI Engine Zonal Simulator		
HSWT Reactor Property	Specifies the burned mass fraction value at which the entire wall heat loss will be switched from the unburned zone to the burned zone. <a href="#">HSWM</a> , <a href="#">HSWT</a> , and <a href="#">HSWC</a> are mutually exclusive.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Temperature</i>	Required	K	HSWM <b>0.05</b>
	Keyword Usage	Optional keyword.		
	Reactor Models	• SI Engine Zonal Simulator		
HSWM Reactor Property	Specifies the burned mass fraction value at which the entire wall heat loss will be switched from the unburned zone to the burned zone. <a href="#">HSWM</a> , <a href="#">HSWT</a> , and <a href="#">HSWC</a> are mutually exclusive.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Burned mass fraction</i>	Required	--	HSWM <b>973.15</b>
	Keyword Usage	Optional keyword.		
	Reactor Models	• SI Engine Zonal Simulator		

Keyword	Definition			
HTC  Reactor Property	The overall, per-area, heat-transfer coefficient for convective or conductive heat transfer out of the system. This keyword is only relevant when the energy equation is being solved.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Material name</i>	<b>Optional.</b>  If no material is specified, the same value will be used for all materials.	--	HTC <b>material1</b> 1.E-4
	<i>Heat transfer coefficient</i>	Required	cal/(cm <sup>2</sup> -K-sec)	HTC material1 <b>1.E-4</b>
	<i>Reactor number (PSR clusters only)</i>	<b>Optional.</b>  If no number is given, the keyword is assumed to apply to all reactors in a cluster.	--	HTC material1 1.E-4 <b>1</b>
	<b>Keyword Usage</b>	Optional keyword. This keyword must be used with TAMB. By default, the heat loss from the reactor will be zero. See also <a href="#">QLOS</a> and <a href="#">QPRO</a> .		
	<b>Reactor Models</b>	<ul style="list-style-type: none"> <li>• Closed Homogeneous Batch Reactor</li> <li>• Closed Plasma Reactor</li> <li>• Honeycomb Monolith Reactor</li> <li>• IC HCCI Engine</li> <li>• Multi-Zone HCCI Engine</li> <li>• Non-reactive Gas Mixer</li> <li>• Perfectly Stirred Reactor (PSR)</li> </ul>		

Keyword	Definition			
		<ul style="list-style-type: none"><li>• Plasma PSR</li><li>• Plasma Plug Flow Reactor</li><li>• Plug Flow Reactor</li><li>• SI Engine Zonal Simulator</li></ul>		
<b>HTCPRO</b>  Reactor Property Profiles	The profile of the overall heat transfer coefficient for convective or conductive heat transfer out of the system. Each <b>HTCPRO</b> entry represents a point in a piecewise-linear profile. The keyword is only relevant when the energy equation is being solved.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Time or Distance value (depending on Reactor Model)</i>	Required	sec or cm	HTCPRO <b>5.0E-5</b> 2.0
	<i>Heat transfer coefficient per area</i>	Required	cal/cm <sup>2</sup> -K-sec	HTCPRO 5.0E-5 <b>2.0</b>
	<i>Reactor number (PSR clusters only)</i>	Optional  If no number is given, the profile described by the first two values is assumed to apply to all reactors in a cluster.	--	HTCPRO 5.0E-5 2.0 <b>1</b>
	<b>Keyword Usage</b>	Optional keyword. By default, there is no heat loss from the reactor. See also <b>HTC</b> , <b>QLOS</b> , <b>HTRN</b> , and <b>QFUN</b> .		
	<b>Reactor Models</b>	<ul style="list-style-type: none"><li>• Closed Homogeneous Batch Reactor</li><li>• Closed Plasma Reactor</li><li>• Cylindrical Shear Flow Reactor</li><li>• Honeycomb Reactor</li><li>• IC HCCI Engine</li><li>• Multi-Zone HCCI Engine</li><li>• Non-reactive Gas Mixer</li></ul>		



Keyword	Definition			
	<ul style="list-style-type: none"> <li>• Perfectly Stirred Reactor (PSR)</li> <li>• Planar Shear Flow Reactor</li> <li>• Plasma PSR</li> <li>• Plasma Plug Flow Reactor</li> <li>• Plug Flow Reactor</li> <li>• SI Engine Zonal Simulator</li> </ul>			
<b>HTRN</b>  Reactor Property	The heat transfer coefficient and ambient temperature for specification of the heat loss from the reactor along the external surface area, at an optionally specified surface material. This keyword is only relevant when the energy equation is being solved.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Material name (0-D and Plug Flow systems only)</i>	Optional  If no material is specified, the same value will be used for all materials.	--	HTRN <b>material1</b> 1.E-4 298
	<i>Heat transfer coefficient</i>	Required	cal/(cm <sup>2</sup> · K · sec)	HTRN <b>1.E-4</b> 298 HTRN <b>1.E-4</b>
	<i>Ambient temperature (0-D and Plug Flow systems only)</i>	Required	K	HTRN 1.E-4 <b>298</b>
	<i>Reactor number (PSR clusters only)</i>	Optional  If no number is given, the keyword is assumed to apply to all reactors in a cluster.	--	HTRN material1 1.E-4 298 <b>1</b>

Keyword	Definition			
	Keyword Usage	Optional keyword. By default, the heat loss from the reactor will be zero. See also <a href="#">QLOS</a> and <a href="#">QPRO</a> .		
	Reactor Models	<ul style="list-style-type: none"><li>• Closed Homogeneous Batch Reactor</li><li>• Closed Plasma Reactor</li><li>• Cylindrical Shear Flow Reactor</li><li>• Honeycomb Reactor</li><li>• Non-reactive Gas Mixer</li><li>• Perfectly Stirred Reactor (PSR)</li><li>• Planar Shear Flow Reactor</li><li>• Plasma Plug Flow Reactor</li><li>• Plasma PSR</li><li>• Plug Flow Reactor</li></ul>		
ICHF Inlet Property	Use the wall function heat transfer correlation to compute the wall heat loss rate for the internal-combustion engine models. For more information about this heat transfer correlation, see the <a href="#">Chemkin-Pro Theory Manual</a> .			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Dimensionless temperature inside turbulent thermal boundary layer</i>	Required.	--	ICHF <b>100.0</b> 0.125 400.00
	<i>Exponent of the viscosity ratio</i>	Required	--	ICHF 100.0 <b>0.125</b> 400.0
	<i>Wall temperature</i>	Required	K	ICHF 100.0 0.125 <b>400.0</b>
	Keyword Usage	Optional keyword.		
	Reactor Models	<ul style="list-style-type: none"><li>• Multi-Zone HCCI Simulator</li><li>• IC HCCI Engine</li><li>• SI Engine Zonal Simulator</li></ul>		
ICHH Reactor Property	Use the Hohenberg formulation to calculate cylinder wall heat transfer coefficient.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>parameter_a</i>	Required	--	ICHH <b>130.0</b> -0.06 0.8 -0.4 1.4 400.0
	<i>parameter_b</i>	Required	--	ICHH 130.0 <b>-0.06</b> 0.8 -0.4 1.4 400.0
	<i>parameter_c</i>	Required	--	ICHH 130.0 -0.06 <b>0.8</b> -0.4 1.4 400.0

Keyword	Definition			
	<i>parameter_d</i>	Required	--	ICHH 130.0 -0.06 0.8 <b>-0.4</b> 1.4 400.0
	<i>parameter_e</i>	Required	m/s	ICHH 130.0 -0.06 0.8 -0.4 <b>1.4</b> 400.0
	<i>ambient_temperature</i>	Required	K	ICHH 130.0 -0.06 0.8 -0.4 1.4 <b>400.0</b>
	<b>Keyword Usage</b>	This keyword is optional and works with IC engine models only. All IC engine heat transfer coefficient options (ICHT, ICHX, ICHW, ICHH, HTC, HTCPRO, and QFUN) are mutually exclusive.  Default: the Hohenberg heat transfer coefficient formulation is NOT used.		
	<b>Reactor Models</b>	<ul style="list-style-type: none"><li>• Closed Homogeneous Batch Reactor</li><li>• Closed Plasma Reactor</li><li>• Cylindrical Shear Flow Reactor</li><li>• Honeycomb Reactor</li><li>• IC HCCI Engine</li><li>• Multi-Zone HCCI Engine</li><li>• Non-reactive Gas Mixer</li><li>• Perfectly Stirred Reactor (PSR)</li><li>• Planar Shear Flow Reactor</li><li>• Plasma Plug Flow Reactor</li><li>• Plasma PSR</li><li>• Plug Flow Reactor</li><li>• SI Engine Zonal Simulator</li></ul>		
<b>ICEN</b>  Reactor Property	The transient internal combustion (IC) HCCI engine model will be implemented. The solution will be obtained with the volume as a function of time, where the function of time is determined by an engine model that defines the volume as a function of user-specified engine parameters. The equations solved are those of a specified volume function of time, but the user does not need to provide a subroutine or volume vs. time profile for this calculation. This problem type is only allowed for closed (zero flow-rate) systems.			
	<b>Keyword Usage</b>	Optional keyword. By default, a constant pressure, constant volume, steady-state problem is assumed.		
	<b>Reactor Models</b>	<ul style="list-style-type: none"><li>• IC HCCI Engine</li></ul>		
	<b>Notes</b>	<ul style="list-style-type: none"><li>• See also: <a href="#">CMPR</a>, <a href="#">VOLC</a>, <a href="#">RPM</a>, and <a href="#">LOLR</a> keywords.</li></ul>		

Keyword	Definition			
		• SI Engine Zonal Simulator		
ICHT  Reactor Property	Convective heat transfer correlation for the transient IC HCCI Engine model, using the following generalized convective heat transfer correlation: $Nu_h=aRe^bPr^c$ . Where $Nu_h$ is the Nusselt number for heat transfer, Re is the Reynolds number, and Pr is the Prandtl number. For more information on the usage of these parameters, see <a href="#">Internal Combustion Engine Model</a> of the <a href="#">Chemkin-Pro Theory Manual</a> .			
	Parameters	Optional/Reqd.	Units	Examples
	The value <i>a</i> in heat transfer correlation	Required	dimensionless	ICHT .035 .5 .33 10. 350.
	The value <i>b</i> in heat transfer correlation	Required	dimensionless	ICHT .035 .5 .33 100 350.
	The value <i>c</i> in heat transfer correlation	Required	dimensionless	ICHT .035 .5 .33 10. 350.
	Bore diameter	Required	cm	ICHT .0350.5 .33 10. 350.
	Wall temperature	Required	K	ICHT .035 .5 .33 10. 350.
	Keyword Usage	Optional keyword. By default, an adiabatic (zero heat loss) condition is assumed. See also <a href="#">GVEL</a> for Woschni correlation extensions.		
	Reactor Models	• IC HCCI Engine  • SI Engine Zonal Simulator		
ICHW  Reactor Property	Use the dimensional Woschni formulation to calculate cylinder wall heat transfer coefficient.			
	Parameters	Optional/Reqd.	Units	Examples
	parameter_a	Required	--	ICHW 3.26 0.8 -0.53 400.0
	parameter_b	Required	--	ICHW 3.26 0.8 -0.53 400.0
	parameter_c	Required	--	ICHW 3.26 0.8 -0.53 400.0
	ambient_temperature	Required	K	ICHW 3.26 0.8 -0.53 400.0
	Keyword Usage	This keyword is optional and works with IC engine models only. All IC engine heat transfer coefficient options (ICHT, ICHX, ICHW, ICHH, HTC, HTCPRO, and QFUN) are mutually exclusive. By default, the dimensional Woschni heat transfer coefficient formulation is NOT used.		
	Reactor Models	• Closed Homogeneous Batch Reactor  • Closed Plasma Reactor		

Keyword	Definition			
		<ul style="list-style-type: none"><li>• Cylindrical Shear Flow Reactor</li><li>• Honeycomb Reactor</li><li>• Non-reactive Gas Mixer</li><li>• Perfectly Stirred Reactor (PSR)</li><li>• Planar Shear Flow Reactor</li><li>• Plasma Plug Flow Reactor</li><li>• Plasma PSR</li><li>• Plug Flow Reactor</li></ul>		
<b>ICRD</b>  Reactor Model or Reactor Property	Flag to specify coordinate system, which determines the Reactor Model and symmetry assumptions for shear-layer flow.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Coordinate flag indicating Planar Shear Flow Reactor, with, non-symmetric boundary conditions</i>	Required	--	ICRD <b>PLAN</b>
	<i>Coordinate flag indicating Planar Shear Flow Reactor, assuming symmetry with respect to the center axis</i>	Required	--	ICRD <b>SYMC</b>
	<i>Coordinate flag indicating Cylindrical Shear Flow Reactor, using radial coordinates</i>	Required	--	ICRD <b>RAD</b>
	<b>Keyword Usage</b>	Required keyword.		
	<b>Reactor Models</b>	<ul style="list-style-type: none"><li>• Cylindrical Shear Flow Reactor</li><li>• Planar Shear Flow Reactor</li></ul>		
	<b>Notes</b>	<ul style="list-style-type: none"><li>• Only one-half of the physical domain is used for the radial or symmetric channel case, and the lower boundary is the symmetry line</li></ul>		
<b>IEM</b>  Reactor Property	Flag indicating that the interaction-by-exchange-with-the-mean (IEM) model will be used to simulate the molecular mixing within the computational particle.			

Keyword	Definition			
	<b>Keyword Usage</b>	Optional keyword. By default, a well mixed model is assumed.		
	<b>Reactor Models</b>	<ul style="list-style-type: none"><li>• Closed Partially Stirred Reactor (PaSR)</li><li>• Partially Stirred Reactor (PaSR)</li></ul>		
<b>IG-RID-METH-OD_n</b>  Reactor Property	Choice for the initial grid profile. Integer <i>n</i> can be 1, 2, or 3 and mean uniform grid, biased grid, and read from an input file, respectively. In general, the uniform grid is not very useful and a biased grid should be used. The bias is created with respect to the location of the stoichiometric mixture fraction.			
	<b>Keyword Usage</b>	Required keyword. The default value is IGRIDMETHOD_2, indicating a biased grid.		
	<b>Reactor Models</b>	<ul style="list-style-type: none"><li>• Diffusion Flamelet Generator</li></ul>		
<b>INIT</b>  Reactor Property	The initial gas mole fraction of the given species in the reactor for a transient simulation. There may be as many <b>INIT</b> lines as there are species in the problem.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Species name</i>	Required	--	INIT <b>N20.79</b>
	<i>Gas fraction</i>	Required	Mole fraction	INIT N2 <b>0.79</b>
	<b>Keyword Usage</b>	Optional keyword. By default, if no <b>INIT</b> entries are made, the inlet gas properties will be used. When some <b>INIT</b> entries are present, species not explicitly entered are taken as having a mole fraction of 0.		
	<b>Reactor Models</b>	<ul style="list-style-type: none"><li>• Closed Partially Stirred Reactor (PaSR)</li><li>• Partially Stirred Reactor (PaSR)</li><li>• Normal Incident Shock</li><li>• Normal Reflected Shock</li><li>• Rotating Disk CVD Reactor</li><li>• Stagnation Flow CVD Reactor</li></ul>		
<b>IN-JM</b>  Reactor Property	Total mass flow rate of the injected gas. See <a href="#">Equation 14.5</a> of the <a href="#">Chemkin-Pro Theory Manual</a> .			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Mass flow rate</i>	Required	g/(cm <sup>2</sup> · sec)	INJM <b>0.15</b>
	<b>Keyword Usage</b>	Required keyword when <b>INJS</b> is used; otherwise it is ignored.		
	<b>Reactor Models</b>	<ul style="list-style-type: none"><li>• Rotating Disk CVD Reactor</li><li>• Stagnation Flow CVD Reactor</li></ul>		

Keyword	Definition			
INJS  Reactor Property	Injection of gas species at a location along the axis of symmetry can be included using one or more <a href="#">INJS</a> keywords. The injection is specified as a spatially distributed Gaussian source. <a href="#">INJM</a> is the total mass flow, i.e., the spatial integral of the mass flow function. This source term will be added to <a href="#">Equation 14.5</a> of the <a href="#">Chemkin-Pro Theory Manual</a> . <a href="#">INJS</a> specifies the species composition of the injected flow, in mole fractions.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Species name</i>	Required	--	INJS <b>H20.5</b>
	<i>Species composition</i>	Required	mole fractions	INJS H2 <b>0.5</b>
	<b>Keyword Usage</b>	Optional keyword. By default, there is no mass injection along the flow axis.		
	<b>Reactor Models</b>	<ul style="list-style-type: none"><li>Rotating Disk CVD Reactor</li><li>Stagnation Flow CVD Reactor</li></ul>		
IN-JT  Reactor Property	Temperature of the injected gas.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Temperature</i>	Required	K	INJT <b>300.</b>
	<b>Keyword Usage</b>	Optional keyword. By default, no enthalpy is added to the energy equation with the injected gas. If <a href="#">INJS</a> is not included, this keyword will be ignored.		
	<b>Reactor Models</b>	<ul style="list-style-type: none"><li>Rotating Disk CVD Reactor</li><li>Stagnation Flow CVD Reactor</li></ul>		
IN-JW  Reactor Property	Half-width of the Gaussian gas-injection source. See <a href="#">Equation 14.5</a> of the <a href="#">Chemkin-Pro Theory Manual</a> .			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Half-width</i>	Required	cm	INJW <b>0.07</b>
	<b>Keyword Usage</b>	Optional keyword. By default, the width is 0.0. Keyword is ignored unless <a href="#">INJS</a> is present.		
	<b>Reactor Models</b>	<ul style="list-style-type: none"><li>Rotating Disk CVD Reactor</li><li>Stagnation Flow CVD Reactor</li></ul>		
IN-JX  Reactor Property	Height above the disk which is the center of the Gaussian-shaped injection source. See <a href="#">Equation 14.5</a> of the <a href="#">Chemkin-Pro Theory Manual</a> .			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Height</i>	Required	cm	INJX <b>0.6</b>
	<b>Keyword Usage</b>	Optional keyword. By default, the height is 0.0. Keyword is ignored unless <a href="#">INJS</a> is present.		
	<b>Reactor Models</b>	<ul style="list-style-type: none"><li>Rotating Disk CVD Reactor</li><li>Stagnation Flow CVD Reactor</li></ul>		

Keyword	Definition			
IN-LET  Reactor Property	Specification of a reactor inlet stream. Specify an optional name for the stream and a reactor number. For each INLET stream defined, you must also specify the corresponding inlet temperature ( TINL), composition ( REAC), or set of EQUI / OXID / FUEL / CPROD / ADD ), and flow rate ( FLRT or SCCM).			
	Parameters	Optional/Reqd.	Units	Examples
	Inlet stream name	Required	--	INLET <b>secondary_air2</b>
	Reactor number (PSR clusters only)	Optional  If no number is given, values are assumed to apply to all reactors in a cluster.	--	INLET secondary_air <b>2</b>
	Keyword Usage	Optional keyword. If no streams are defined, the program will assume there is a single inlet for the first reactor in series or that the system is a single closed reactor (if FLRT, SCCM and TAU are not defined).		
	Reactor Models	<ul style="list-style-type: none"><li>• Diffusion or Premixed Opposed-flow Flame</li><li>• Non-reactive Gas Mixer</li><li>• Partially Stirred Reactor (PaSR)</li><li>• Perfectly Stirred Reactor (PSR)</li><li>• Plasma PSR</li><li>• Rotating Disk CVD Reactor</li><li>• Stagnation Flow CVD Reactor</li></ul>		
	Notes	<ul style="list-style-type: none"><li>• This keyword can not be changed for a restart or continuation run.</li></ul>		
INTM  Reactor Property	The estimated peak mole fractions values for “intermediate” species. One of these INTM inputs should appear for each intermediate species desired. It is usually better to estimate values somewhat higher than those that are actually present in the flame. For example, INTM HO2 0.001 gives an estimate fraction of 0.001 for the intermediate HO2. Any given species can participate simultaneously as a reactant, intermediate, or product.			
	Parameters	Optional/Reqd.	Units	Examples
	Species name	Required	--	INTM <b>HO20.001</b>



Keyword	Definition			
	<i>Estimated fraction</i>	Required	mole fraction	INTM HO2 <b>0.001</b>
	<b>Keyword Usage</b>	Optional keyword. By default, the estimated fraction is set to 0 unless the user has set a minimum threshold to a non-zero value on the Reactor panel (see <a href="#">XIMN</a> to set a non-zero threshold value).		
	<b>Reactor Models</b>	<ul style="list-style-type: none"><li>• Premixed Laminar Burner-stabilized Flame</li><li>• Premixed Laminar Flame-speed Calculation</li><li>• Rotating Disk CVD Reactor</li><li>• Stagnation Flow CVD Reactor</li></ul>		
	<b>Notes</b>	<ul style="list-style-type: none"><li>• See <a href="#">Starting Estimates</a> of the <a href="#">Chemkin-Pro Theory Manual</a> for more information.</li></ul>		
<b>IONE</b>  Reactor Property	Specified energy loss to ions in the sheath for each ion lost at a specified material. The energy that the ions gain in the sheath is specified in electron Volts. For example, "IONE material1 30" would result in an ion energy gain of 30 eV as it crossed the sheath near the material <i>material1</i> . This energy gain for the ions results in a reduced effective power deposition to the electrons (unless <a href="#">ELSH</a> is also specified), as described in <a href="#">Electron Energy Equation for Plasma Systems</a> of the <a href="#">Chemkin-Pro Theory Manual</a> .			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Material name</i>	Optional  If there is no material name than the specified energy loss applies to all materials.	--	IONE <b>material1</b> 30 1
	<i>Specified energy loss</i>	Required	eV	IONE <b>30</b>
	<i>Reactor number (PSR clusters only)</i>	Optional  If no number is given, values are assumed to apply	--	IONE material1 30 <b>1</b>

Keyword	Definition			
		to all reactors in a cluster.		
	Keyword Usage	Optional keyword. By default, the ion energy is determined by the <a href="#">ELSH</a> keyword.		
	Reactor Models	<ul style="list-style-type: none"><li>• Closed Plasma Reactor</li><li>• Plasma Plug Flow Reactor</li><li>• Plasma PSR</li></ul>		
IPSR	Use this keyword to specify which PSR to use for the initialization ( <a href="#">XMLI</a> ), when more than one PSR is stored on the XML Solution File that is used for initialization (i.e. on <i>XMLdata.zip</i> ).			
XMLI	Parameters	Optional/Reqd.	Units	Examples
	<i>PSR number</i>	Required	--	IPSR <b>2</b>
	Keyword Usage	Optional keyword. By default, the last PSR saved in the XML Solution File is used.		
	Reactor Models	<ul style="list-style-type: none"><li>• Chemical and Phase Equilibrium Calculations</li><li>• Closed Homogeneous Batch Reactor</li><li>• Closed Plasma Reactor</li><li>• Cylindrical Shear Flow Reactor</li><li>• Diffusion or Premixed Opposed-flow Flame</li><li>• Honeycomb Reactor</li><li>• IC HCCI Engine</li><li>• Mechanism Analyzer</li><li>• Non-reactive Gas Mixer</li><li>• Normal Incident Shock</li><li>• Normal Reflected Shock</li><li>• Perfectly Stirred Reactor (PSR)</li><li>• Planar Shear Flow Reactor</li><li>• Plasma Plug Flow Reactor</li><li>• Plasma PSR</li><li>• Plug Flow Reactor</li><li>• Premixed Laminar Burner-stabilized Flame</li></ul>		

Keyword	Definition			
		<ul style="list-style-type: none"><li>• Premixed Laminar Flame-speed Calculation</li><li>• Rotating Disk CVD Reactor</li><li>• SI Engine Zonal Simulator</li><li>• Stagnation Flow CVD Reactor</li></ul>		
IRET Solver	Number of time steps to be taken in <i>Twopnt</i> 's pseudo time stepping algorithm before increasing the time step.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Number of time steps</i>	Required	--	IRET <b>200</b>
	Keyword Usage	Optional keyword. By default, the number of times steps is set to 25 or 50 depending on the Reactor Model (See Notes below).		
	Reactor Models	<ul style="list-style-type: none"><li>• Cylindrical Shear Flow Reactor</li><li>• Diffusion or Premixed Opposed-flow Flame</li><li>• Non-reactive Gas Mixer</li><li>• Perfectly Stirred Reactor (PSR)</li><li>• Planar Shear Flow Reactor</li><li>• Premixed Laminar Burner-stabilized Flame</li><li>• Premixed Laminar Flame-speed Calculation</li><li>• Plasma PSR</li><li>• Rotating Disk CVD Reactor</li><li>• Stagnation Flow CVD Reactor</li></ul>		
	Notes	<ul style="list-style-type: none"><li>• Default value is 25 for PSRs and 50 for all other reactors listed above.</li></ul>		
ISHK Problem Type	Inclusion of this keyword designates an incident shock problem without boundary layer correction.			
	Keyword Usage	Required keyword. Either <a href="#">ISHK</a> or <a href="#">ISKB</a> must be included to indicate a Normal Incident Shock problem type. See also <a href="#">RSHK</a> .		
	Reactor Models	<ul style="list-style-type: none"><li>• Normal Incident Shock</li></ul>		
ISKB Problem Type	Inclusion of this keyword designates an incident shock problem with boundary layer correction.			

Keyword	Definition			
	<b>Keyword Usage</b>	Required keyword. Either <b>ISHK</b> or <b>ISKB</b> must be included to indicate a Normal Incident Shock problem type. See also <b>RSHK</b> .		
	<b>Reactor Models</b>	<ul style="list-style-type: none"><li>Normal Incident Shock</li></ul>		
<b>ISTP</b> Solver	specifies the number of initial pseudo time steps that are taken by the steady-state TWOPNT solver, prior to attempting a Newton iteration. Normally, the Newton iteration will be attempted first, with time steps invoked only if the Newton iteration fails. Nevertheless, there may be circumstances where initial time stepping is desirable. The time step size is specified with the <b>TIM1</b> or <b>TIM2</b> keyword. The <b>ISTP</b> keyword only applies to the first grid network, not the subsequently refined ones. If need to find a steady state solution via pure time integration, please refer to the <b>TRAN</b> option.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Number of initial time steps</i>	Required	--	<b>ISTP 100</b>
	<b>Keyword Usage</b>	Optional keyword. By default, the number of initial time steps is set to 0.		
	<b>Reactor Models</b>	<ul style="list-style-type: none"><li>Cylindrical Shear Flow Reactor</li><li>Diffusion or Premixed Opposed-flow Flame</li><li>Non-reactive Gas Mixer</li><li>Perfectly Stirred Reactor (PSR)</li><li>Planar Shear Flow Reactor</li><li>Plasma PSR</li><li>Premixed Laminar Burner-stabilized Flame</li><li>Premixed Laminar Flame-speed Calculation</li><li>Rotating Disk CVD Reactor</li><li>Stagnation Flow CVD Reactor</li></ul>		
<b>JJRG</b> Restart	On continuations or restarts, the number of mesh points can be reduced. <i>Twopnt</i> itself does not remove grid points. Therefore, on a sequence of continuation problems the number of grid points can grow because the region where they are needed may change. <b>JJRG</b> thus provides a capability to remove grid points. The old solution is adaptively interpolated onto a new grid of <b>JJRG</b> points. When <b>JJRG</b> is added, its effect is carried over to the subsequent continuations, if any. Often this is not desired. To prevent its operation, <b>JJRG</b> can be set to a high value, such as the maximum number of grid-points. The reduction of grid points then does not happen since <b>JJRG</b> does not add grid-points.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Number of mesh points</i>	Required	--	<b>JJRG 40</b>

Keyword	Definition			
	Keyword Usage	Optional keyword. By default, the number of grid points will be the same as in the previous solution.		
	Reactor Models	<ul style="list-style-type: none"><li>• Diffusion or Premixed Opposed-flow Flame</li><li>• Premixed Laminar Burner-stabilized Flame</li><li>• Premixed Laminar Flame-speed Calculation</li><li>• Rotating Disk CVD Reactor</li><li>• Stagnation Flow CVD Reactor</li></ul>		
KLIM  Output	Calculate the ignition delay as the time when the fraction of the specified species reaches its maximum value. Only applicable when you are solving the energy equation with transient solver.			
	Parameters	Optional/Reqd.	Units	Examples
	Species name	Required	--	KLIM <b>OH</b>
	Keyword Usage	Optional keyword. See also <a href="#">TIFP</a> .		
	Reactor Models	<ul style="list-style-type: none"><li>• Closed Homogeneous Batch Reactor</li><li>• Closed Plasma Reactor</li><li>• Honeycomb Monolith Reactor</li><li>• IC HCCI Engine</li><li>• Perfectly Stirred Reactor (PSR)</li><li>• Plasma PSR</li><li>• Plasma Plug Flow Reactor</li><li>• Plug Flow Reactor</li><li>• SI Engine Zonal Simulator</li></ul>		
KNMN  Reactor Property	The minimum Knudsen number, above which the wall slip-velocity model will be used.			
	Parameters	Optional/Reqd.	Units	Examples
	Minimum Knudsen number	Required	--	KNMN <b>10</b>
	Keyword Usage	Optional keyword. It is relevant only when the slip velocity model is used. See also <a href="#">SLIP</a> .		
	Reactor Models	<ul style="list-style-type: none"><li>• Cylindrical Shear Flow Reactor</li><li>• Planar Shear Flow Reactor</li></ul>		

Keyword	Definition			
<b>KOUT</b>  Output	List of species names whose mass fractions will be printed to the diagnostic output file for Premixed or Opposed-flow Flames or to the <i>history.plt</i> file for PaSRs. A maximum number of 5 species can be included on a single line.			
	Parameters	Optional/Reqd.	Units	Examples
	List of species names	Required	--	KOUT <b>H2 O2 H2O H OH</b>
	<b>Keyword Usage</b>	Optional keyword. By default, none of the species fractions are printed.		
	<b>Reactor Models</b>	<ul style="list-style-type: none"><li>• Diffusion or Premixed Opposed-flow Flame</li><li>• Closed Partially Stirred Reactor (PaSR)</li><li>• Partially Stirred Reactor (PaSR)</li><li>• Premixed Laminar Burner-stabilized Flame</li><li>• Premixed Laminar Flame-speed Calculation</li></ul>		
<b>LG-DT</b>  Solver	Controls the time interval for data to be written to the XML Solution File (e.g., <i>XMLdata.zip</i> ) using a logarithmic time scale.			
	Parameters	Optional/Reqd.	Units	Examples
	Logarithmic time-step	Required	ALOG10(sec)	LGDT <b>1.0</b>
	<b>Keyword Usage</b>	Optional keyword. If neither <b>DTSV</b> nor <b>LGDT</b> are set, then the time step used is ending time minus the beginning time, divided by 100.		
	<b>Reactor Models</b>	<ul style="list-style-type: none"><li>• Normal Incident Shock</li><li>• Normal Reflected Shock</li></ul>		
<b>LINE</b>  Reactor Property	An indicator that a linear profile is used for the initial gas species distribution along the reactor center line. For Opposed-flow Flames, the mole fractions vary linearly from one inlet to the other, with inlet values forming the end points. For transient CVD Reactors, the mole fractions vary linearly from the inlet values, specified by keyword <b>REAC</b> , to the <b>INIT</b> value at the surface.			
	<b>Keyword Usage</b>	Optional keyword. By default, a plateau profile is used for Opposed-flow Flames ( <b>PLAT</b> ). For transient CVD Reactors, the default initial gas species profiles are assumed axially uniform with mole fractions specified by <b>INIT</b> ; the keyword is ignored for steady-state CVD Reactor simulations.		
	<b>Reactor Models</b>	<ul style="list-style-type: none"><li>• Rotating Disk CVD Reactor</li><li>• Stagnation Flow CVD Reactor</li></ul>		
<b>LMLM</b>	Minimum amount of liquid mass to activate the vaporization model.			

Keyword	Definition			
Reactor Property/Model	Parameters	Optional/Reqd.	Units	Examples
	<i>Minimum total liquid mass</i>	Required	g	LMLM <b>1.0E-7</b>
	<b>Keyword Usage</b>	Optional keyword. Default is 1.0E-8 g.		
	<b>Reactor Models</b>	• Direct Injection Diesel Engine Simulator		
LO-DR  Reactor Property	Piston offset to crank radius ratio.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Ratio of piston offset to crank radius.</i>	Required	None	LODR <b>0.1</b>
	<b>Keyword Usage</b>	Optional keyword. Default = 0.0.		
	<b>Reactor Models</b>	• IC HCCI Engine  • Multi-zone HCCI Engine  • SI Engine Zonal Simulator		
	<b>Notes</b>	• The absolute value of LODR must be less than the value of LOLR minus 1.0:   LODR  < (LOLR - 1).		
LOLR  Reactor Property	Ratio of the length of the engine connecting rod to the crank radius.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Connection rod to crank radius ratio</i>	Required	--	LOLR <b>5.</b>
	<b>Keyword Usage</b>	Optional keyword. By default, this ratio is 33.3.		
	<b>Reactor Models</b>	• IC HCCI Engine  • SI Engine Zonal Simulator		
LPRT  Output	Printing control <b>LPRT</b> turns on extensive printing that provides information on rates of progress of individual surface reactions. This can be informative in understanding the surface reaction behavior.			
	<b>Keyword Usage</b>	Optional keyword. By default, there is no extended printing of surface rate information.		
	<b>Reactor Models</b>	• Rotating Disk CVD Reactor  • Stagnation Flow CVD Reactor		
LSCL  Reactor Property	Sets the length scale (cm) for the calculation of gas and surface Damkohler numbers.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Length scale</i>	Required	cm	LSCL <b>3.</b>
	<b>Keyword Usage</b>	Optional keyword. By default, the length scale is 1 cm.		

Keyword	Definition			
	Reactor Models	• Mechanism Analyzer		
LUMP-TO  Reactor Property	This is an optional approach to species mass conservation closure. In this case, the selected species is assumed to be a diluent and its fraction is set to one minus the sum of all others			
	Parameters	Optional/Reqd.	Units	Examples
	Species name	Required	--	LUMPTO AR
	Keyword Usage	Optional keyword.		
	Reactor Models	• Cylindrical Shear Flow Reactor  • Planar Shear Flow Reactor		
MAJ  Reactor Property	Sets the “Major Species”. This is only used to calculate an effective diffusion coefficient when non-dimensionalizing the reaction rate constants.			
	Parameters	Optional/Reqd.	Units	Examples
	Species name	Optional	--	MAJ CH4
	Species number	Optional	--	MAJ 1
	Keyword Usage	Optional keyword. The default is to use the gas species with the second largest mole fraction (from the XBTH input) in the bath-gas composition. If the gas-phase bath-gas composition is not specified, the default is to use the second species in the mechanism.		
	Reactor Models	• Mechanism Analyzer		
MAXIT  Solver	Controls the maximum number of iterations the integrator solver can take per step to solve the transient problem. The default is 4 and you should increase this value to give the integrator greater chance to solve your problem if it is very hard to solve (stiff or very nonlinear or discontinuous) or if the run fails with a “nonlinear solver failed to converge repeatedly” message.			
	Parameters	Optional/Reqd.	Units	Examples
	Iteration number	Required	--	MAXIT 10
	Keyword Usage	Optional keyword.		
	Reactor Models	• Closed Homogeneous Batch Reactor  • Closed Partially Stirred Reactor  • Closed Plasma Reactor  • Cylindrical Shear Flow Reactor  • Honeycomb Reactor  • IC HCCI Engine  • Multi-Zone HCCI Engine Simulator  • Partially Stirred Reactor (PaSR)		



Keyword	Definition			
		<ul style="list-style-type: none"><li>• Perfectly Stirred Reactor (PSR)</li><li>• Planar Shear Flow Reactor</li><li>• Plasma Plug Flow Reactor</li><li>• Plasma PSR</li><li>• Plug Flow Reactor</li><li>• Rotating Disk CVD Reactor</li><li>• SI Engine Zonal Simulator</li><li>• Stagnation Flow CVD Reactor</li></ul>		
<b>MAX-TIME</b>  Solver	The maximum number times the steady state solver TWOPNT will use its pseudo-time stepping algorithm. You may need to increase this value for very stiff problems to allow TWOPNT to find a solution by letting it switch between steady state searching and time stepping more than 100 times.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Maximum steady state iterations</i>	Optional	--	MAXTIME <b>200</b>
	<b>Keyword Usage</b>	Optional keyword. By default, the maximum number of time stepping operations is 100.		
	<b>Reactor Models</b>	<ul style="list-style-type: none"><li>• Cylindrical Shear Flow Reactor</li><li>• Diffusion or Premixed Opposed-flow Flame</li><li>• Non-reactive Gas Mixer</li><li>• Perfectly Stirred Reactor (PSR)</li><li>• Planar Shear Flow Reactor</li><li>• Plasma PSR</li><li>• Premixed Laminar Burner-stabilized Flame</li><li>• Premixed Laminar Flame-speed Calculation</li><li>• Rotating Disk CVD Reactor</li><li>• Stagnation Flow CVD Reactor</li></ul>		
	<b>Notes</b>	<ul style="list-style-type: none"><li>• SSMAXITER must be &gt;=1.</li></ul>		
<b>MCUT</b>  Reactor Property	Minimum number of particles required to “switch on” the surface rate calculations (coagulation and surface reaction). The default value is 1 [particles/cm <sup>3</sup> ].			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Material name</i>	Required	--	MCUT <b>C(B)</b> 100

Keyword	Definition			
	<i>Cutoff number density</i>	Required	particles/cm <sup>3</sup>	MCUT C(B) <b>100</b>
	<b>Keyword Usage</b>	Optional keyword.		
	<b>Reactor Models</b>	<ul style="list-style-type: none"><li>• Closed Homogeneous Batch Reactor</li><li>• Closed Plasma Reactor</li><li>• Cylindrical Shear Flow Reactor</li><li>• Honeycomb Monolith Reactor</li><li>• IC HCCI Engine</li><li>• Perfectly Stirred Reactor (PSR)</li><li>• Planar Shear Flow Reactor</li><li>• Plasma PSR</li><li>• Plasma Plug Flow Reactor</li><li>• Plug Flow Reactor</li><li>• SI Engine Zonal Simulator</li></ul>		
<b>MIX</b>	Use a mixture-average model for calculating the transport coefficients and diffusion fluxes.			
Reactor Property	<b>Keyword Usage</b>	Optional keyword. By default, mixture-averaged transport is used.		
	<b>Reactor Models</b>	<ul style="list-style-type: none"><li>• Cylindrical Shear Flow Reactor</li><li>• Diffusion or Premixed Opposed-flow Flame</li><li>• Planar Shear Flow Reactor</li><li>• Premixed Laminar Burner-stabilized Flame</li><li>• Premixed Laminar Flame-speed Calculation</li><li>• Rotating Disk CVD Reactor</li><li>• Stagnation Flow CVD Reactor</li></ul>		
<b>MIX</b>	Flag indicating a mixing-only problem, where chemistry will be ignored.			
Reactor Property	<b>Keyword Usage</b>	Optional keyword. This is the default. See also <a href="#">CHEM</a> and <a href="#">EQUI</a> .		
	<b>Reactor Models</b>	<ul style="list-style-type: none"><li>• Closed Partially Stirred Reactor (PaSR)</li><li>• Partially Stirred Reactor (PaSR)</li></ul>		

Keyword	Definition			
MIX-FRAC-BIAS_FUEL  Reactor Property	Bias factor for the grid on the fuel side, that is, between the mixture fraction equal to its stoichiometric mixture fraction and 1. A value greater than unity should be given and it means more grid points near the stoichiometric mixture fraction.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Bias factor for grid</i>	Required for corresponding grid choice.	--	MIXFRACBIAS_FUEL 1.2
	Keyword Usage	Required keyword.		
	Reactor Models	• Diffusion Flamelet Generator		
MIX-FRAC-BIAS_OX-ID  Reactor Property	Bias factor for the grid on the oxidizer side, that is, between the mixture fraction equal to its stoichiometric mixture fraction and 0. A value greater than unity should be given and it means more grid points near the stoichiometric mixture fraction.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Bias factor for grid</i>	Required for corresponding grid choice.	--	MIXFRACBIAS_OXID 1.2
	Keyword Usage	Required keyword.		
	Reactor Models	• Diffusion Flamelet Generator		
MIXT  Reactor Property	The characteristic time of the mixing process in the reactor.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Characteristic time</i>	Required	sec	MIXT 1.0E-3
	Reactor Models	• Closed Partially Stirred Reactor (PaSR)  • Partially Stirred Reactor (PaSR)		
MLMT  Solver	Specifies the minimum value of gas mass in the zones. By default, the minimum zone mass is set to 10 <sup>-6</sup> g.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Value of the b parameter</i>	Optional	--	MLMT 1.0E-5
	Keyword Usage	Optional keyword.		
	Reactor Models	• SI Engine Zonal Simulator		
MMASS  MMASS	The reactor wall temperature will be obtained by solving energy conservation equation for the reactor wall. It uses the thermal mass of the reactor wall and the heat transfer coefficient between the inner wall surface and the gas mixture inside the reactor. MMASS specifies the thermal mass of the reactor wall.			

Keyword	Definition			
	Parameters	Optional/Reqd.	Units	Examples
	Material name	<b>Optional.</b> If no material is specified, the same value will be used for all materials.	--	MMASS <b>material1</b> 500
	Thermal mass	Required	cal/K	MMASS <b>500</b>
	Reactor number (PSR clusters only)	<b>Optional.</b> If no number is given, the keyword is assumed to apply to all reactors in a cluster.	--	MMASS material1.500 <b>1</b>
	Keyword Usage	Optional keyword. This keyword must be used with <a href="#">GMHTC</a> . For Plug Flow Reactors the unit of thermal mass is cal/(cm-K).		
	Reactor Models	<ul style="list-style-type: none"><li>• Closed Homogeneous Batch Reactor</li><li>• Closed Plasma Reactor</li><li>• Honeycomb Monolith Reactor</li><li>• IC HCCI Engine</li><li>• Non-reactive Gas Mixer</li><li>• Perfectly Stirred Reactor (PSR)</li><li>• Plasma PSR</li><li>• Plasma Plug Flow Reactor</li><li>• Plug Flow Reactor</li><li>• SI Engine Zonal Simulator</li></ul>		
MO-MEN	Turn on or off solution of the momentum equation for a plug-flow simulation.			
	Parameters	Optional/Reqd.	Units	Examples

Keyword	Definition			
Reactor Property	<i>String "ON" or "OFF" to toggle the momentum equation</i>	Required	--	MOMEN <b>ON</b>  MOMEN OFF
	<b>Keyword Usage</b>	Optional keyword. By default, the momentum equation is solved (ON).		
	<b>Reactor Models</b>	<ul style="list-style-type: none"><li>• Honeycomb Reactor</li><li>• Plasma Plug Flow Reactor</li><li>• Plug Flow Reactor</li></ul>		
<b>MORD</b>  Solver	Maximum order of integration used by the transient solver.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Maximum order of integration</i>	Required	--	MORD <b>3</b>
	<b>Keyword Usage</b>	Optional keyword. By default, the maximum order of integration is 5.		
	<b>Reactor Models</b>	<ul style="list-style-type: none"><li>• Cylindrical Shear Flow Reactor</li><li>• Planar Shear Flow Reactor</li><li>• Rotating Disk CVD Reactor</li><li>• Stagnation Flow CVD Reactor</li></ul>		
<b>MQA-FR</b>  Reactor Property	The external heat transfer (heat loss) area fraction of each zone.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Area fraction</i>	Required	--	MQAFR 0.15 4
	<i>Zone number</i>	Required	--	MQAFR 0.15 4
	<b>Keyword Usage</b>	Optional keyword.		
	<b>Reactor Models</b>	<ul style="list-style-type: none"><li>• Multi-Zone HCCI Engine Simulator</li></ul>		
<b>MS-FX</b>  Reactor Property	Use a new discretization scheme for convective flux terms. In some cases, the original discretization scheme might not conserve species fluxes across the flame zone. With this new scheme, species mass fluxes are always conserved. Since accurate mass fluxes require fine resolution of species profiles, this new scheme in general incurs more grid points and longer run time than the original scheme does. The differences between major species solutions obtained by these two schemes are subtle.			
	<b>Keyword Usage</b>	Optional keyword. By default, the original discretization scheme is used.		
	<b>Reactor Models</b>	<ul style="list-style-type: none"><li>• Premixed Laminar Burner-stabilized Flame</li><li>• Premixed Laminar Flame-speed Calculation</li></ul>		

Keyword	Definition			
MULT  Reactor Property	Use full multicomponent model for the transport coefficients and diffusion fluxes. See also <a href="#">MIX</a> .			
	Keyword Usage	Optional keyword. By default, mixture-averaged transport is used.		
	Reactor Models	<ul style="list-style-type: none"><li>• Cylindrical Shear Flow Reactor</li><li>• Diffusion or Premixed Opposed-flow Flame</li><li>• Planar Shear Flow Reactor</li><li>• Premixed Laminar Burner-stabilized Flame</li><li>• Premixed Laminar Flame-speed Calculation</li><li>• Rotating Disk CVD Reactor</li><li>• Stagnation Flow CVD Reactor</li></ul>		
MV-FAC  Reactor Property/Model	Artificial scaling factor to modify the vaporization rates.			
	Parameters	Optional/Reqd.	Units	Examples
	Scaling factor	Required	--	MVFAC <b>0.9</b>
	Keyword Usage	Optional keyword. Default is 1.0.		
	Reactor Models	<ul style="list-style-type: none"><li>• Direct Injection Diesel Engine Simulator</li></ul>		
MXITS  Reactor Property/Model	The maximum number of iterations allowed to solve for the droplet surface temperature. This parameter is associated with the “Solve for Surface T” option of the vaporization model.			
	Parameters	Optional/Reqd.	Units	Examples
	Number of iterations	Required	--	MXITS <b>100</b>
	Keyword Usage	Optional keyword. Default is 50.		
	Reactor Models	<ul style="list-style-type: none"><li>• Direct Injection Diesel Engine Simulator</li></ul>		
MZMAS  Reactor Property	Specifies zone mass fractions. MZM will compute the exact zone volumes at the beginning of the simulation. Use either <a href="#">VOL</a> or <a href="#">MZMAS</a> to set up the initial zone volumes: An error will be issued if both keywords are used in the same input file.			
	Parameters	Optional/Reqd.	Units	Examples
	zone mass fraction	Required		MZMAS <b>0.2 7</b>
	zone number	Required		MZMAS 0.2 <b>7</b>
	Keyword Usage	Optional keyword.		
	Reactor Models	<ul style="list-style-type: none"><li>• Multi-Zone HCCI Engine Simulator</li></ul>		
NADAP  Solver	Turns off the saving of adaptive points (see <a href="#">ADAP</a> , which is the default). NADAP is provided to turn off adaptive points during a continuous run if they have already been turned on with <a href="#">ADAP</a> .			

Keyword	Definition			
	Keyword Usage	Optional keyword. By default, <b>ADAP</b> is the default in the ANSYS Chemkin-Pro user interface and <b>NADAP</b> is the default for the command line.		
	Reactor Models	<ul style="list-style-type: none"><li>• Closed Plasma Reactor</li><li>• Closed Homogeneous Reactor</li><li>• Honeycomb Reactor</li><li>• IC HCCI Engine Model</li><li>• Multi-Zone HCCI Engine Simulator</li><li>• Plasma Plug Flow Reactor</li><li>• Plug Flow Reactor</li><li>• SI Engine Zonal Simulator</li></ul>		
<b>NADP</b> Reactor Property	Number of mesh points that <i>Twopt</i> can add at one time during each grid refinement.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Number of mesh points</i>	Required	--	<b>NADP 2</b>
	Keyword Usage	Optional keyword. By default, no maximum is set for the number of points that can be added at once by the <i>Twopt</i> solver.		
	Reactor Models	<ul style="list-style-type: none"><li>• Diffusion or Premixed Opposed-flow Flame</li><li>• Premixed Laminar Burner-stabilized Flame</li><li>• Premixed Laminar Flame-speed Calculation</li><li>• Rotating Disk CVD Reactor</li><li>• Stagnation Flow CVD Reactor</li></ul>		
	Notes	<ul style="list-style-type: none"><li>• This keyword can not be changed on a continuation or restart run.</li></ul>		
<b>NCANG</b> Reactor Property	Run the simulation for 180 degrees of crank angle (0.5 revolution). If the “starting crank angle” (DEG0) is set to 180 degrees, the simulation will stop at crank angle = 360 (=180+180) degrees (i.e., top dead center). Use one of <b>TIME</b> , <b>NREV</b> , or <b>NCANG</b> to set the simulation time. The last keyword (of the three) in the input file takes effect.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>number_of_crank_angles</i>	Required	degrees	<b>NCANG 180</b>
	Keyword Usage	Optional keyword.		
	Reactor Models	<ul style="list-style-type: none"><li>• IC HCCI Engine</li></ul>		

Keyword	Definition			
		• SI Engine Zonal Simulator		
NCFIT  Reactor Property	Optional number of time points used to determine the slope when used in conjunction with keyword <a href="#">CTOL</a> .			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Number of time points</i>	Required	--	NCFIT <b>100</b>
	<b>Keyword Usage</b>	Optional keyword. NCFIT is only used in conjunction with <a href="#">CTOL</a> .		
		• Closed Partially Stirred Reactor (PaSR)  • Partially Stirred Reactor (PaSR)		
	<b>Notes</b>	Default value is 100.		
ND-PR  Output or Solver	Frequency of output printing during time integration, given as the number of time steps.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Print frequency</i>	Required	--	NDPR <b>50</b>
	<b>Keyword Usage</b>	Optional keyword. By default, the print frequency is at every 1 time step.		
	<b>Reactor Models</b>	• Closed Partially Stirred Reactor (PaSR)  • Diffusion or Premixed Opposed-flow Flame  • Partially Stirred Reactor (PaSR)		
	NE-WRUN  Reactor Property	Inclusion of this keyword causes ANSYS Chemkin-Pro to expect keywords for another problem to follow the END keyword. The following problem does not use the solution of the previous problem as its initial guess. This capability is quite different to that provided by <a href="#">CNTN</a> . The solutions resulting from NEWRUN keywords are written sequentially to one XML Solution File.		
<b>Keyword Usage</b>		Optional keyword. By default, no new run is expected.		
<b>Reactor Models</b>		• Chemical and Phase Equilibrium Calculations  • Closed Homogeneous Batch Reactor  • Closed Plasma Reactor  • Cylindrical Shear Flow Reactor  • Honeycomb Monolith Reactor  • IC HCCI Engine  • Mechanism Analyzer  • Non-reactive Gas Mixer  • Normal Incident Shock		



Keyword	Definition			
		<ul style="list-style-type: none"><li>• Normal Reflected Shock</li><li>• Partially Stirred Reactor</li><li>• Perfectly Stirred Reactor (PSR)</li><li>• Planar Shear Flow Reactor</li><li>• Plasma PSR</li><li>• Plasma Plug Flow Reactor</li><li>• Plug Flow Reactor</li><li>• Rotating Disk CVD Reactor Using Transient Solver</li><li>• SI Engine Zonal Simulator</li><li>• Stagnation Flow CVD Reactor Using Transient Solver</li></ul>		
<b>NINT-G-STEPS</b>  Reactor Property	The number of internal steps that the solver can take. When the integration time is too long and/or the system of equations is too stiff, the solver may take many internal time steps. This control acts as a check to avoid long, infinite, or hung processes. The simulator may take a corrective action (such as trying a few more steps or declare failure and/or provide diagnostic information).			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Maximum value of SSDR</i>	Optional	--	NINTGSTEPS <b>10000</b>
	<b>Keyword Usage</b>	Optional keyword. The default value for the Diffusion Flamelet Generator is 5000.		
	<b>Reactor Models</b>	<ul style="list-style-type: none"><li>• Diffusion Flamelet Generator</li></ul>		
<b>NJAC</b>  Solver	For the steady-state <i>TwoPnt</i> solver, specifies the maximum number of Newton steps that can be taken in solving the steady state problem before a new Jacobian is evaluated. If NJAC=1, then a full Newton method will result.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Retirement age</i>	Required	--	NJAC <b>20</b>
	<b>Keyword Usage</b>	Optional keyword. By default, the retirement age is set at 20.		
	<b>Reactor Models</b>	<ul style="list-style-type: none"><li>• Cylindrical Shear Flow Reactor</li><li>• Diffusion or Premixed Opposed-flow Flame</li><li>• Non-reactive Gas Mixer</li><li>• Perfectly Stirred Reactor (PSR)</li><li>• Planar Shear Flow Reactor</li><li>• Plasma PSR</li></ul>		

Keyword	Definition			
		<ul style="list-style-type: none"><li>• Premixed Laminar Burner-stabilized Flame</li><li>• Premixed Laminar Flame-speed Calculation</li><li>• Rotating Disk CVD Reactor</li><li>• Stagnation Flow CVD Reactor</li></ul>		
NMOM  Reactor Property	Number of moments used in the simulation for tracking particle size distribution. MINMO(=3) ≤ NMOM ≤ MAXMO(=6). If NMOM = 6, then 6 moments of the size distribution function are solved, from the 0 <sup>th</sup> moment to the 5 <sup>th</sup> moment.			
	Parameters	Optional/Reqd.	Units	Examples
	Number of moments	Required	--	NMOM <b>6</b>
	Keyword Usage	Optional keyword. Default is the MINMO value.		
	Reactor Models	<ul style="list-style-type: none"><li>• Closed Homogeneous Batch Reactor</li><li>• Closed Plasma Reactor</li><li>• Cylindrical Shear Flow Reactor</li><li>• Honeycomb Monolith Reactor</li><li>• IC HCCI Engine</li><li>• Perfectly Stirred Reactor (PSR)</li><li>• Planar Shear Flow Reactor</li><li>• Plasma PSR</li><li>• Plasma Plug Flow Reactor</li><li>• Plug Flow Reactor</li><li>• SI Engine Zonal Simulator</li></ul>		
NNEG  Solver	Flag instructing transient solver to try to constrain all components of the solution vector to be non-negative. This is usually unnecessary, but it may help to use this keyword if negative solution components appear to be causing problems in convergence.			
	Keyword Usage	Optional keyword. By default, the solution is not constrained and is not usually necessary.		
	Reactor Models	<ul style="list-style-type: none"><li>• Closed Homogeneous Batch Reactor</li><li>• Closed Partially Stirred Reactor (PaSR)</li><li>• Closed Plasma Reactor</li><li>• Honeycomb Reactor</li></ul>		

Keyword	Definition			
		<ul style="list-style-type: none"><li>• IC HCCI Engine</li><li>• Non-reactive Gas Mixer</li><li>• Partially Stirred Reactor (PaSR)</li><li>• Perfectly Stirred Reactor (PSR)</li><li>• Plasma PSR</li><li>• Plasma Plug Flow Reactor</li><li>• Plug Flow Reactor</li><li>• SI Engine Zonal Simulator</li></ul>		
	Notes	• <b>NNEG</b> can be added to but cannot be removed from a continuation run.		
<b>NO-AGG</b>  Reactor Property	Turns off particle aggregation effect. Particle aggregation is included by default in the Particle Tracking module.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Material name</i>	Required	--	NOAGG <b>SOOT</b>
	Keyword Usage	Optional keyword.		
	Reactor Models	<ul style="list-style-type: none"><li>• Closed Homogeneous Batch Reactor</li><li>• Closed Plasma Reactor</li><li>• Diffusion or Premixed Opposed-flow Flame</li><li>• IC HCCI Engine</li><li>• Multi-Zone HCCI Engine Simulator</li><li>• Perfectly Stirred Reactor (PSR)</li><li>• Plasma PSR</li><li>• Premixed Laminar Burner-stabilized Flame</li></ul>		
<b>NOCG</b>  Reactor Property	Exclude coagulation of particles.			
	Keyword Usage	Optional keyword.		
	Reactor Models	<ul style="list-style-type: none"><li>• Closed Homogeneous Batch Reactor</li><li>• Closed Plasma Reactor</li><li>• Cylindrical Shear Flow Reactor</li><li>• Honeycomb Monolith Reactor</li><li>• IC HCCI Engine</li></ul>		

Keyword	Definition	
		<ul style="list-style-type: none"> <li>• Perfectly Stirred Reactor (PSR)</li> <li>• Planar Shear Flow Reactor</li> <li>• Plasma PSR</li> <li>• Plasma Plug Flow Reactor</li> <li>• Plug Flow Reactor</li> <li>• SI Engine Zonal Simulator</li> </ul>
<b>NOCH</b>  Reactor Property	This keyword specifies that the rates of all gas-phase reactions will be set to zero, regardless of the values specified in the <i>Gas-phase Kinetics</i> input.	
	<b>Keyword Usage</b>	Optional keyword. By default, gas chemistry is turned on. See also <a href="#">CHEM</a> .
	<b>Reactor Models</b>	<ul style="list-style-type: none"> <li>• Rotating Disk CVD Reactor</li> <li>• Stagnation Flow CVD Reactor</li> </ul>
<b>NOFT</b>  Solver or Reactor Property	For steady-state cases, when this keyword is specified and an energy equation is being solved, the intermediate solution at a fixed temperature will be skipped. In this case, solution to the energy and species equations will be attempted simultaneously from the user-specified initial guess.	
	<b>Keyword Usage</b>	Optional keyword. By default, the fixed temperature solution is obtained before adding the energy equation.
	<b>Reactor Models</b>	<ul style="list-style-type: none"> <li>• Diffusion or Premixed Opposed-flow Flame</li> <li>• Non-reactive Gas Mixer</li> <li>• Perfectly Stirred Reactor (PSR)</li> <li>• Plasma PSR</li> <li>• Premixed Laminar Burner-stabilized Flame</li> <li>• Premixed Laminar Flame-speed Calculation</li> <li>• Rotating Disk CVD Reactor</li> <li>• Stagnation Flow CVD Reactor</li> </ul>
	<b>Notes</b>	• See also, <a href="#">ENRG</a> and <a href="#">ENGE</a> keywords.
<b>NO-JC</b>  Solver	Flag indicating the non-stiff Adams method (no Jacobian) of the DVODE solver is used to integrate the equations.	
	<b>Keyword Usage</b>	Optional keyword. By default, the DASPK solver will be used.
	<b>Reactor Models</b>	<ul style="list-style-type: none"> <li>• Closed Partially Stirred Reactor (PaSR)</li> </ul>

Keyword	Definition			
		• Partially Stirred Reactor (PaSR)		
NONE Output	Turns default output off for all of <i>Surftherm</i> 's tables. One can use this keyword in combination with another keyword below, to turn on output from only a few features. This keyword will also turn off all previously specified output from keywords given before it.			
	Keyword Usage	Optional keyword. By default, the <b>ALL</b> output will be printed.		
	Reactor Models	• Mechanism Analyzer		
NONR Reactor Property	This keyword specifies that the non-reacting problem will not be solved as the first stage in the solution of the full problem.			
	Keyword Usage	Optional keyword. By default, the non-reacting problem is solved first.		
	Reactor Models	• Rotating Disk CVD Reactor  • Stagnation Flow CVD Reactor		
NOTP Reactor Property	Exclude thermophoresis of particles.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Material name</i>	Required	--	NOTP <b>SOOT</b>
	Keyword Usage	Optional keyword. By default, thermophoresis of particles is excluded.		
	Reactor Models	• Diffusion or Premixed Opposed-flow Flame  • Opposed-flow Flame  • Premixed Laminar Burner-stabilized Flame  • Premixed Laminar Flame-speed Calculation		
NOTP Solver	Do not solve for the initial gas-phase and surface concentrations at the walls using the <i>Twopnt</i> procedure.			
	Keyword Usage	Optional keyword. By default, the initial <i>Twopnt</i> procedure is solved.		
	Reactor Models	• Cylindrical Shear Flow Reactor  • Planar Shear Flow Reactor		
NPAR Reactor Property	The number of statistical events (particles) used by the Monte Carlo process to form the stochastic ensemble.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Number of particles</i>	Required	--	NPAR <b>1000</b>
	Keyword Usage	Required keyword.		
	Reactor Models	• Closed Partially Stirred Reactor (PaSR)		

Keyword	Definition			
		• Partially Stirred Reactor (PaSR)		
NP_FUEL  Reactor Property	Number of points on the fuel side, that is, between the mixture fraction equal to its stoichiometric mixture fraction and 1.			
	Parameters	Optional/Reqd.	Units	Examples
	Number of grid points	Required for corresponding grid choice	--	NP_FUEL 11
	Keyword Usage	Required keyword.		
	Reactor Models	• Diffusion Flamelet Generator		
NP_OX-ID  Reactor Property	Number of points on the oxidizer side, that is, between the mixture fraction equal to its stoichiometric mixture fraction and 0.			
	Parameters	Optional/Reqd.	Units	Examples
	Number of grid points	Required for corresponding grid choice	--	NP_OXID 11
	Keyword Usage	Required keyword.		
	Reactor Models	• Diffusion Flamelet Generator		
NPIN  Reactor Property	The minimum number of event particles in the reactor whose properties will be replaced by those of the inlet mixture per time step.			
	Parameters	Optional/Reqd.	Units	Examples
	Number of particles	Required	--	NPIN 5
	Keyword Usage	Optional keyword. By default, the minimum number of the event particles is 2.		
	Reactor Models	• Partially Stirred Reactor (PaSR)		
NPSR  Reactor Property	Number of perfectly stirred reactors (PSRs) or zones in a reactor cluster.			
	Parameters	Optional/Reqd.	Units	Examples
	Number of reactors or zones	Required	--	NPSR 5
	Keyword Usage	Optional keyword. By default, the number of PSRs is set to 1.		
		• Non-reactive Gas Mixer  • Perfectly Stirred Reactor (PSR)  • Plasma PSR		

Keyword	Definition			
NPTS  Reactor Property	The number of initial mesh points. The inclusion of NPTS will generate an equi-spaced mesh of NPTS points across the domain, in the axial direction for Flames and CVD Reactors, and in the cross-flow direction for Shear Flow Reactors. The user can also specify an initial non-uniform mesh using the keyword GRID, in which case the NPTS input is not needed.			
	Parameters	Optional/Reqd.	Units	Examples
	Number of mesh points	Required	--	NPTS 50
	Keyword Usage	Optional keyword. By default, the number of initial mesh points is set to 6.		
	Reactor Models	<ul style="list-style-type: none"><li>• Cylindrical Shear Flow Reactor</li><li>• Diffusion or Premixed Opposed-flow Flame</li><li>• Planar Shear Flow Reactor</li><li>• Premixed Laminar Burner-stabilized Flame</li><li>• Premixed Laminar Flame-speed Calculation</li><li>• Rotating Disk CVD Reactor</li><li>• Stagnation Flow CVD Reactor</li></ul>		
NREV  Reactor Property	The number of revolutions of the crank used to determine the end time of the simulation. Fractional values are acceptable.			
	Parameters	Optional/Reqd.	Units	Examples
	Number of revolutions	Required	--	NREV 1
	Keyword Usage	Optional keyword. Either NREV or TIME must be specified.		
	Reactor Models	<ul style="list-style-type: none"><li>• IC HCCI Engine</li><li>• SI Engine Zonal Simulator</li></ul>		
NSOL  XMLI	Use this keyword to specify which solution to use for the initialization ( XMLI) or restart ( RSTR), when more than one solution is stored on the XML Solution File that is used for the restart or initialization (e.g., on XMLdata.zip).			
	Parameters	Optional/Reqd.	Units	Examples
	Solution used	Required	--	NSOL 3
	Keyword Usage	Optional keyword. By default, the last solution saved in the XML Solution File.		
	Reactor Models	<ul style="list-style-type: none"><li>• Chemical and Phase Equilibrium Calculations</li><li>• Closed Homogeneous Batch Reactor</li></ul>		

Keyword	Definition														
	<ul style="list-style-type: none"> <li>• Closed Plasma Reactor</li> <li>• Cylindrical Shear Flow Reactor</li> <li>• Diffusion or Premixed Opposed-flow Flame</li> <li>• Honeycomb Reactor</li> <li>• IC HCCI Engine</li> <li>• Mechanism Analyzer</li> <li>• Non-reactive Gas Mixer</li> <li>• Normal Incident Shock</li> <li>• Normal Reflected Shock</li> <li>• Perfectly Stirred Reactor (PSR)</li> <li>• Planar Shear Flow Reactor</li> <li>• Plasma Plug Flow Reactor</li> <li>• Plasma PSR</li> <li>• Plug Flow Reactor</li> <li>• Premixed Laminar Burner-stabilized Flame</li> <li>• Premixed Laminar Flame-speed Calculation</li> <li>• Rotating Disk CVD Reactor</li> <li>• SI Engine Zonal Simulator</li> <li>• Stagnation Flow CVD Reactor</li> </ul>														
<b>NSTEPS_HIGH</b> Reactor Property	<p>Number of steps to be taken to reach the specified maximum value of SSDR (SSDR_max). The simulator computes the new SSDR to be taken on a subsequent step as SSDR used in previous step + fixedStepSize where the fixedStepSize = (SSDR_max - SSDR_Nominal)/NSTEPS_High. For example, if the specified nominal and maximum values are 1 and 21, respectively, then 5 steps will yield the constant size to be 4 and result in the sequence of SSDR values as {1, 5, 9, 13, 17, 21}.</p> <p>Continuations to the maximum value can be turned off by setting this input to 0.</p> <table> <tr> <th>Parameters</th><th>Optional/Reqd.</th><th>Units</th><th>Examples</th></tr> <tr> <td>Number of steps to maximum SSDR</td><td>Required</td><td>--</td><td>NSTEPS_HIGH 5</td></tr> <tr> <td><b>Keyword Usage</b></td><td colspan="3">Required keyword.</td></tr> </table>			Parameters	Optional/Reqd.	Units	Examples	Number of steps to maximum SSDR	Required	--	NSTEPS_HIGH 5	<b>Keyword Usage</b>	Required keyword.		
Parameters	Optional/Reqd.	Units	Examples												
Number of steps to maximum SSDR	Required	--	NSTEPS_HIGH 5												
<b>Keyword Usage</b>	Required keyword.														



Keyword	Definition			
	Reactor Models	• Diffusion Flamelet Generator		
NSTEPS_LOW  Reactor Property	Number of steps to be taken to reach the specified minimum value of SSDR. The simulator computes the new SSDR to be used on a subsequent step as a constantFactor * SSDR_Used_in_previous step. That is, NSTEP_LOW* log(constantFactor) = log(SSDR_min/SSDR_nominal). For example, if the specified nominal and minimum values are 1 and 0.001, respectively, then 3 steps will yield the constant factor to be 0.1 and result in the sequence of SSDR values as {1, 0.1, 0.01, 0.001}.			
	Continuations to the minimum value can be turned off by setting this input to 0.			
	Parameters	Optional/Reqd.	Units	Examples
	Number of steps to maximum SSDR	Required	--	NSTEPS_HIGH 5
	Keyword Usage	Required keyword.		
	Reactor Models	• Diffusion Flamelet Generator		
NTOT  Reactor Property	Maximum number of grid points allowed during mesh adaptation.			
	Parameters	Optional/Reqd.	Units	Examples
	Number of grid points	Required	--	NTOT 200
	Keyword Usage	Optional keyword. The default maximum number of grid points is 100 for: Rotating Disk CVD Reactor, Stagnation Flow CVD Reactor; 250 for Diffusion or Premixed Opposed-flow Flame, Premixed Laminar Burner-stabilized Flame, Premixed Laminar Flame-speed Calculation.		
	Reactor Models	• Diffusion or Premixed Opposed-flow Flame  • Premixed Laminar Burner-stabilized Flame  • Premixed Laminar Flame-speed Calculation  • Rotating Disk CVD Reactor  • Stagnation Flow CVD Reactor		
	Notes	• This keyword can not be changed on a restart or continuation run.  • In previous versions, NMAX keyword was used.		
NZCDC  Inlet Property	Discharge coefficient of the injector.			
	Parameters	Optional/Reqd.	Units	Examples
	Injector name	Required	--	NZCDC modelX 0.68
	Discharge coefficient	Required	--	NZCDC modelX 0.68

Keyword	Definition			
	Keyword Usage	Required keyword.		
	Reactor Models	• Direct Injection Diesel Engine Simulator		
NZDIA	Diameter of the nozzle hole of the injector.			
Inlet Property	Parameters	Optional/Reqd.	Units	Examples
	Injector name	Required	--	NZDIA <b>modelX</b> 0.037
	Diameter	Required	--	NZDIA modelX <b>0.037</b>
	Keyword Usage	Required keyword.		
	Reactor Models	• Direct Injection Diesel Engine Simulator		
NZHOL	Number of nozzle holes in the injector.			
Inlet Property	Parameters	Optional/Reqd.	Units	Examples
	Injector name	Required	--	NZHOL <b>injector1</b> 8
	Number of holes	Required	--	NZHOL injector1 <b>8</b>
	Keyword Usage	Required keyword.		
	Reactor Models	• Direct Injection Diesel Engine Simulator		
NZINJ	Number of injections from the injector.			
Inlet Property	Parameters	Optional/Reqd.	Units	Examples
	Injector name	Required	--	NZINJ <b>stock1</b> 2
	Number of injections	Required	--	NZINJ stock1 <b>2</b>
	Keyword Usage	Required keyword.		
	Reactor Models	• Direct Injection Diesel Engine Simulator		
NZLDR	Nozzle hole length to diameter ratio of the injector.			
Inlet Property	Parameters	Optional/Reqd.	Units	Examples
	Injector name	Required	--	NZLDR <b>modelX</b> 4.0
	Length to diameter ratio	Required	--	NZLDR modelX <b>4.0</b>
	Keyword Usage	Required keyword.		
	Reactor Models	• Direct Injection Diesel Engine Simulator		
NZONE	Specifies the number of zones to be used in the multi-zone simulation. This keyword MUST be used with the <b>ICEN</b> keyword or an error will be issued. The default value is 1 (= single zone model). The multi-zone model will be turned on when <b>NZONE</b> > 1.			
Reactor Property	Parameters	Optional/Reqd.	Units	Examples
	Number of zones	Required	--	NZONE <b>5</b>
	Keyword Usage	Optional keyword.		
	Reactor Models	• Multi-Zone HCCI Engine Simulator		

Keyword	Definition			
NZRDR  Inlet Property	Ratio of the radius of the inside rounded corner to the nozzle diameter of the injector.			
	Parameters	Optional/Reqd.	Units	Examples
	Injector name	Required	--	NZRDR <b>injector1</b> 0.06
	Corner radius to diameter ratio	Required	--	NZRDR injector1 <b>0.06</b>
	Keyword Usage	Required keyword.		
	Reactor Models	• Direct Injection Diesel Engine Simulator		
NZR-WL  Inlet Property	The characteristic distance from the nozzle to the cylinder wall or the piston head. When the spray parcel penetration distance is greater than this value, the wall-impingement submodel will be activated. The wall-impingement model will adjust the speed and the average droplet diameter of the spray parcel. The model assumes all liquid mass will rebound back to the cylinder volume.			
	Parameters	Optional/Reqd.	Units	Examples
	Injector name	Required	--	NZRWL <b>injector1</b> 6.0
	Nozzle distance	Required	cm	NZRWL injector1 <b>6.0</b>
	Keyword Usage	Optional keyword. Default is 1.0E6.		
	Reactor Models	• Direct Injection Diesel Engine Simulator		
OINL  Reactor Property	The inlet-gas spin rate. At the inlet $x=L$ , $v/r = \text{OINL}$ .			
	Parameters	Optional/Reqd.	Units	Examples
	Inlet-gas spin rate	Required	rpm	OINL <b>100</b>
	Keyword Usage	Optional keyword. By default, the inlet-gas spin rate is 0.0.		
	Reactor Models	• Rotating Disk CVD Reactor		
OMEG  Problem Type and Reactor Property	The disk rotation rate; also specifies the Rotating Disk CVD Reactor model.			
	Parameters	Optional/Reqd.	Units	Examples
	Disk rotation rate	Required	rpm	OMEG <b>1000</b>
	Keyword Usage	Required keyword. See also <a href="#">STAG</a> .		
	Reactor Models	• Rotating Disk CVD Reactor		
OX-ID  Inlet or Reactor Property	Defines the oxidizer mole fraction composition for an inlet stream in an open system, or for the initial conditions in a closed system, when an equivalence ratio is specified ( <a href="#">EQUI</a> ). It must be followed by a species name and then the mole fraction. One of these <a href="#">OXID</a> inputs must appear for each oxidizer species, which are used to determine the inlet composition based on an equivalence-ratio calculation ( <a href="#">EQUI</a> ). Any given species can participate simultaneously as a fuel, oxidizer, or product. The sum of all the oxidizer mole fractions should equal one. If it does not, a warning message will be printed and the mole fractions will be normalized so the sum does equal one.			
	Parameters	Optional/Reqd.	Units	Examples

Keyword	Definition			
	<i>Inlet stream name (PSRs only)</i>	Optional  If there is no stream name than the oxidizer mole fraction composition applies to the default or all defined streams.	--	OXID <b>mixture1</b> O2 0.5
	<i>Species name</i>	Required	--	OXID <b>O2</b> 0.5
	<i>Fuel fraction</i>	Required	mole fractions	OXID O2 <b>0.5</b>
	<b>Keyword Usage</b>	Required keyword when <a href="#">EQUI</a> option is used for an inlet stream or for the initial conditions in a reactor.		
	<b>Reactor Models</b>	<ul style="list-style-type: none"> <li>• Closed Homogeneous Batch Reactor</li> <li>• Honeycomb Reactor</li> <li>• IC HCCI Engine</li> <li>• Perfectly Stirred Reactor</li> <li>• Plasma Plug Flow Reactor</li> <li>• Plasma PSR</li> <li>• Plug Flow Reactor</li> <li>• SI Engine Zonal Simulator</li> </ul>		
	<b>Notes</b>	<ul style="list-style-type: none"> <li>• The mole fractions are of the oxidizer itself, not for the entire composition.</li> <li>• The <a href="#">OXID</a> keywords must be changed as a set, not individually for a restart run.</li> <li>• The <a href="#">OXID</a> keywords must be changed as a set, not individually for continuation run.</li> </ul>		

## 10.3. Alphabetical Listing of Keywords [P-S]

**Table 10.3: Alphabetical Listing of Keywords [P-S]**

Keyword	Definition			
<b>P1A</b>  Reactor Property	Pressure before the incident shock.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Pressure</i>	Required	atm	P1A <b>1.0</b>
	<b>Keyword Usage</b>	Optional Keyword. The shock velocity and any two of temperature, pressure, or density must be specified for conditions before the incident shock. See also <a href="#">T1</a> and <a href="#">RHO1</a> .		
	<b>Reactor Models</b>	<ul style="list-style-type: none"><li>• Normal Incident Shock</li><li>• Normal Reflected Shock</li></ul>		
<b>P2A</b>  Reactor Property	Pressure after the incident shock.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Pressure</i>	Required	atm	P2A <b>2.3</b>
	<b>Keyword Usage</b>	Optional Keyword. Any two of temperature, pressure, or density must be specified for conditions after the incident shock. See also <a href="#">T2</a> and <a href="#">RHO2</a> .		
	<b>Reactor Models</b>	<ul style="list-style-type: none"><li>• Normal Incident Shock</li><li>• Normal Reflected Shock</li></ul>		
<b>P3A</b>  Reactor Property	Pressure after the reflected shock, given as $p_5$ in the equations.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Pressure</i>	Required	atm	P3A <b>2.3</b>
	<b>Keyword Usage</b>	Optional Keyword. Any two of temperature, pressure, or density must be specified for conditions before the reflected shock. See also <a href="#">T3</a> and <a href="#">RHO3</a> .		
	<b>Reactor Models</b>	<ul style="list-style-type: none"><li>• Normal Reflected Shock</li></ul>		
<b>PARP</b>  Output	Partial-pressures of the gas-phase species will be used in the diagnostic output file.			
	<b>Keyword Usage</b>	Optional keyword. By default, mass fractions are printed, not partial pressures.		
	<b>Reactor Models</b>	<ul style="list-style-type: none"><li>• Cylindrical Shear Flow Reactor</li><li>• Planar Shear Flow Reactor</li></ul>		
<b>PB-DEN</b>  Output	This keyword resets all bulk species densities defined in the surface mechanism to the value given by this keyword.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>material_name</i>	Required	None	PBDEN <b>ligA</b> 2.15

Keyword	Definition			
	<i>bulk_density</i>	Required	g/cm <sup>3</sup>	PBDEN ligA <b>2.15</b>
	<b>Keyword Usage</b>	Optional keyword.		
	<b>Reactor Models</b>	<ul style="list-style-type: none"><li>• Closed Homogeneous Reactor</li><li>• Perfectly Stirred Reactor (PSR)</li><li>• Plug Flow Reactor (PFR)</li></ul>		
<b>PDF</b> Output	Request the probability distribution of a scalar to be output to a <i>pdf.plt</i> file. Any number of <b>PDF</b> entries is allowed.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Scalar (temperature or species name)</i>	Required	--	PDF <b>T</b>
	<b>Keyword Usage</b>	Optional keyword. By default, no <b>PDF</b> is printed.		
	<b>Reactor Models</b>	<ul style="list-style-type: none"><li>• Closed Partially Stirred Reactor (PaSR)</li><li>• Partially Stirred Reactor (PaSR)</li></ul>		
<b>PENG</b> Reactor Property	Include the energy conservation equation for particles.			
	<b>Keyword Usage</b>	Optional keyword.		
	<b>Reactor Models</b>	<ul style="list-style-type: none"><li>• Opposed-flow Flame</li><li>• Premixed Laminar Burner-stabilized Flame</li><li>• Premixed Laminar Flame-speed Calculation</li></ul>		
<b>PEST</b> Reactor Property	Specifies an estimate of the equilibrium pressure.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Pressure</i>	Required	atm	PEST <b>1.1</b>
	<b>Keyword Usage</b>	Optional keyword. May help convergence to the equilibrium pressure, or assure an appropriate equilibrium pressure is calculated when a second, trivial solution exists.		
	<b>Reactor Models</b>	<ul style="list-style-type: none"><li>• Chemical and Phase Equilibrium Calculations</li></ul>		
<b>PFAL</b> Output	Analyze the pressure fall-off of a gas phase reaction, i.e., creates a table of reaction rates versus total gas pressure at a constant temperature. The <b>ALL</b> option is the default and produces tables for every gas-phase reaction. The <b>NONE</b> option suppresses output for all of the reactions. If reaction information is desired for only certain reactions, they may be optionally specified by their number (given in the Pre-processor output) or by typing an exact duplicate of the reaction expression (see example input).			
	Parameters	Optional/Reqd.	Units	Examples
	<i>ALL option</i>	<b>Option- al, de-</b>	--	PFAL <b>ALL</b>

Keyword	Definition			
		<b>fault is ALL</b>		
	<i>NONE option</i>	<b>Optional, default is ALL</b>	--	PFAL <b>NONE</b>
	<i>Gas reaction number list</i>	<b>Optional, default is ALL</b>	--	PFAL <b>2 5</b>
	<i>Gas reaction expression</i>	<b>Optional, default is ALL</b>	--	PFAL <b>2CH3(+M)&lt;=&gt;C2H6(+M)</b>
	<b>Keyword Usage</b>	Optional keyword. By default, the table output is determined by the <b>ALL</b> or <b>NONE</b> keyword.		
	<b>Reactor Models</b>	• Mechanism Analyzer		
<b>PFLR</b>	Set the minimum bounds of the particle moments to a slightly negative number to allow the solver more room to search for a solution.			
Reactor Property	Parameters	Optional/Reqd.	Units	Examples
	<i>Minimum bound</i>	Required	--	<b>PFLR -1.0d-06</b>
	<b>Keyword Usage</b>	Optional keyword.		
	<b>Reactor Models</b>	• Opposed-flow Flame  • Premixed Laminar Burner-stabilized Flame  • Premixed Laminar Flame-speed Calculation		
<b>PH</b>	Constant pressure and enthalpy constraints.			
Problem Type	<b>Keyword Usage</b>	Optional keyword. Exactly one problem type keyword must be included.		
	<b>Reactor Models</b>	• Chemical and Phase Equilibrium Calculations		
	<b>Notes</b>	HP keyword is equivalent.		
<b>PHIA</b>	Set the upper limit of the pressure range (in atmospheres) in tables where the gas pressure is varied.			
Reactor Property	Parameters	Optional/Reqd.	Units	Examples
	<i>Pressure</i>	Required	atm	PHIA <b>2.</b>
	<b>Keyword Usage</b>	Optional keyword. By default, the pressure is 1.315789 atm (1000 Torr).		
	<b>Reactor Models</b>	• Mechanism Analyzer		
	<b>Notes</b>	• <b>In previous versions, keyword PHIG was used with units of Torr</b>		

Keyword	Definition			
PLAN  Reactor Property	Use a planar coordinate system, which is appropriate for a Tsuji burner configuration.			
	Keyword Usage	Optional keyword. By default, the coordinate system is radial and axisymmetric.		
	Reactor Models	• Diffusion or Premixed Opposed-flow Flame		
PLAT  Reactor Property	Use a plateau profile to set up initial solution estimates, rather than a linear profile.			
	Keyword Usage	Optional keyword. By default, the plateau profile is used.		
	Reactor Models	• Diffusion or Premixed Opposed-flow Flame		
PLOA  Reactor Property	Set the lower limit of the pressure range (in atmospheres) in tables where the gas pressure is varied.			
	Parameters	Optional/Reqd.	Units	Examples
	Pressure	Required	atm	PLOA <b>1.0</b>
	Keyword Usage	Optional keyword. By default, the pressure is 0.001315789 atm (1 Torr)		
	Reactor Models	• Mechanism Analyzer		
	Notes	• <b>In previous versions, keyword PLOW was used with units of Torr</b>		
PLUG  Reactor Property	Indicates that plug-flow equations will be solved and that the Reactor Model will be one of the family of Plug Flow Reactors.			
	Keyword Usage	Required keyword.		
	Reactor Models	• Honeycomb Reactor  • Plasma Plug Flow Reactor  • Plug Flow Reactor		
PNDE  Reactor Property	Assigns the initial (or estimate for steady-state calculations) number density of the particle consisting of the designated bulk species. The default value is 0. The reactor number is optional. When no reactor number is given, the same initial number density will apply to all reactors in the network. If neither <a href="#">PVFE</a> nor <a href="#">PROE</a> is given, the initial/estimate values of the moments are computed as			
	$M_0 = \text{PNDE}$ $M_i = (\Delta C_{\text{nuc1}}) \times M_{i-1} \quad 1 < i \leq \text{NMOM}$			
	Parameters	Optional/Reqd.	Units	Examples
	Material name	Required	--	PNDE <b>C(B)</b> 1.0E10 4
	Number density	Required	particles/cm <sup>3</sup>	PNDE C(B) <b>1.0E10 4</b>
	Reactor number	Optional	--	PNDE C(B) 1.0E10 <b>4</b>



Keyword	Definition			
	Keyword Usage	Optional keyword. The default value is value for the number density is 0.		
	Reactor Models	<ul style="list-style-type: none"><li>• Closed Homogeneous Batch Reactor</li><li>• Closed Plasma Reactor</li><li>• Cylindrical Shear Flow Reactor</li><li>• Honeycomb Monolith Reactor</li><li>• IC HCCI Engine</li><li>• Perfectly Stirred Reactor (PSR)</li><li>• Planar Shear Flow Reactor</li><li>• Plasma PSR</li><li>• Plasma Plug Flow Reactor</li><li>• Plug Flow Reactor</li><li>• SI Engine Zonal Simulator</li></ul>		
PNDI  Inlet Property	Assigns the number density of the particle consisting of the designated material name to the named inlet stream. The default value is 0. The stream name is optional if there is only one inlet.			
	Parameters	Optional/Reqd.	Units	Examples
	Stream name	Optional if only one inlet.	--	PNDI <b>exhaust</b> C(B) 1.0E12
	Material name	Required	--	PNDI exhaust <b>C(B)</b> 1.0E12
	Mass density	Required	particles/cm <sup>3</sup>	PNDI exhaust C(B) <b>1.0E12</b>
	Keyword Usage	Optional keyword. The default value for the mass density is 0.		
	Reactor Models	<ul style="list-style-type: none"><li>• Cylindrical Shear Flow Reactor</li><li>• Honeycomb Monolith Reactor</li><li>• Perfectly-stirred Reactor (PSR)</li><li>• Planar Shear Flow Reactor</li><li>• Plasma PSR</li><li>• Plasma Plug Flow Reactor</li><li>• Plug-flow Reactor (PFR)</li></ul>		

Keyword	Definition			
<b>PNUM</b>  Reactor Property	Set the total number of pressure entries in tables where the gas pressure is varied. The default is 10. Note that the changes in the pressure are determined on a logarithmic scale.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Number of pressures</i>	Required	--	PNUM <b>10</b>
	<b>Keyword Usage</b>	Optional keyword. By default, the number of pressures is 10.		
	<b>Reactor Models</b>	• Mechanism Analyzer		
<b>PPRO</b>  Reactor Property Profiles	Reactor pressure profile specified as a function of time for transient 0-D homogeneous systems or as a function of distance for Plug Flow Reactors.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Time or Distance value, depending on Reactor Model</i>	Required	sec or cm	PPRO <b>1.0E-4</b> 1.0
	<i>Pressure</i>	Required	atm	PPRO 1.0E-4 <b>1.0</b>
	<i>Reactor number (PSR clusters only)</i>	Optional  If no number is given, the profile described by the first two values is assumed to apply to all reactors in a cluster.	--	PPRO 1.0E-4 1.0 <b>1</b>
	<b>Keyword Usage</b>	Optional keyword. By default, no profile is provided.		
	<b>Reactor Models</b>	• Closed Homogeneous Batch Reactor  • Closed Plasma Reactor  • Diffusion or Premixed Opposed-flow Flame  • Honeycomb Reactor  • Non-reactive Gas Mixer  • Perfectly Stirred Reactor (PSR)  • Plasma Plug Flow Reactor		

Keyword	Definition			
		<ul style="list-style-type: none"><li>• Plasma PSR</li><li>• Plug Flow Reactor</li></ul>		
PRDL  Reactor Property	The Prandlt number used in the generalized heat transfer correlation.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Prandlt number</i>	Required	--	PRDL <b>0.77</b>
	Keyword Usage	Optional keyword. By default, the value is 0.7.		
	Reactor Models	<ul style="list-style-type: none"><li>• IC HCCI Engine</li><li>• SI Engine Zonal Simulator</li></ul>		
PRES  Reactor Property	The reactor pressure in atmospheres. Depending on the Reactor Model and problem type, the pressure specified can serve as the pressure constraint (for constant-pressure problems), as an initial guess for pressure (for steady-state problems where pressure is a variable), or as the initial reactor pressure (for transient cases where pressure is a variable). For the Mechanism Analyzer, this is the bath-gas pressure.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Reactor pressure</i>	Required	atm	PRES <b>1.0</b>
	<i>Reactor number (PSR clusters only)</i>	Optional  If no number is given, the keyword is assumed to apply to all reactors in a cluster.	--	PRES 1.0 <b>1</b>
	Keyword Usage	Required keyword in most cases. Optional keyword only for Mechanism Analyzer, where the default is 1 atm.		
	Reactor Models	<ul style="list-style-type: none"><li>• Chemical and Phase Equilibrium Calculations</li><li>• Closed Homogeneous Batch Reactor</li><li>• Closed Partially Stirred Reactor (PaSR)</li><li>• Closed Plasma Reactor</li><li>• Cylindrical Shear Flow Reactor</li><li>• Diffusion or Premixed Opposed-flow Flame</li></ul>		

Keyword	Definition			
	<ul style="list-style-type: none"><li>• Honeycomb Reactor</li><li>• IC HCCI Engine</li><li>• Mechanism Analyzer</li><li>• Non-reactive Gas Mixer</li><li>• Partially Stirred Reactor (PaSR)</li><li>• Perfectly Stirred Reactor (PSR)</li><li>• Planar Shear Flow Reactor</li><li>• Plasma Plug Flow Reactor</li><li>• Plasma PSR</li><li>• Plug Flow Reactor</li><li>• Premixed Laminar Burner-stabilized Flame</li><li>• Premixed Laminar Flame-speed Calculation</li><li>• Rotating Disk CVD Reactor</li><li>• SI Engine Zonal Simulator</li><li>• Stagnation Flow CVD Reactor</li></ul>			
	<b>Notes</b> <ul style="list-style-type: none"><li>• In previous version, <b>PRMT</b> was an alternate keyword that allowed pressure input in millitorr units, for 0-D homogeneous and plug-flow systems only.</li><li>• In previous versions, this was PBTH for the Mechanism Analyzer.</li></ul>			
<b>PRMN</b> Reactor Property	Minimum mole fraction value applied to the estimated values of the flame products, when the (default) equilibrium is used to determine product estimates. Ignored in the case that <b>PROD2</b> keywords are present.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Product fraction</i>	Required	mole fractions	PRMN <b>1.0E-10</b>
	<b>Keyword Usage</b>	Optional keyword. By default, the flame product fraction is set to 0.		
	<b>Reactor Models</b>	<ul style="list-style-type: none"><li>• Premixed Laminar Burner-stabilized Flame</li><li>• Premixed Laminar Flame-speed Calculation</li></ul>		
<b>PRNT</b> Output	Printing control. “PRNT 0” provides printed output for only the solution (plus sensitivity coefficients and rates-of-production coefficients, when requested). “PRNT 1” provides an additional summary of the iteration path from the solver.			

Keyword	Definition			
	"PRNT 2" includes printing at every stage of the <i>TwoPnt</i> solver's Newton iteration and time stepping procedure. More printing is sometimes helpful when diagnosing problems and trying to adjust the input parameters to optimize convergence. However, since the increased printing requires more function evaluations to show how the solution is progressing, the computer time increases with increased printing.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Print control number</i>	Required	--	PRNT 1
	Keyword Usage	Optional keyword. By default, the print control is set to 1.		
	Reactor Models	<ul style="list-style-type: none"><li>• Closed Homogeneous Batch Reactor</li><li>• Closed Plasma Reactor</li><li>• Cylindrical Shear Flow Reactor</li><li>• Diffusion or Premixed Opposed-flow Flame</li><li>• Honeycomb Reactor</li><li>• IC HCCI Engine</li><li>• Non-reactive Gas Mixer</li><li>• Perfectly Stirred Reactor (PSR)</li><li>• Planar Shear Flow Reactor</li><li>• Plasma Plug Flow Reactor</li><li>• Plasma PSR</li><li>• Plug Flow Reactor</li><li>• Premixed Laminar Burner-stabilized Flame</li><li>• Premixed Laminar Flame-speed Calculation</li><li>• Rotating Disk CVD Reactor</li><li>• SI Engine Zonal Simulator</li><li>• Stagnation Flow CVD Reactor</li></ul>		
PROD	Estimated values of the gas-phase mole fractions at the far end of the domain (i.e., the deposition surface for CVD reactors or the burned state at <a href="#">XEND</a> for Premixed Laminar Flames) or in the middle of the flame (for Opposed-flow Flames). The sum of the product mole fractions should equal to 1.0; if they do not, then a warning message will be printed to the diagnostic output file and the mole fractions will be normalized so that they do sum to one.			
Reactor Property	Parameters	Optional/Reqd.	Units	Examples

Keyword	Definition																							
	Species name	Required	--	PROD <b>H2O</b> 0.5																				
	Mole fraction	Required	--	PROD H2O <b>0.5</b>																				
	Keyword Usage	Optional keyword. If <b>PROD2</b> keywords are not provided, then an equilibrium calculation will be used to determine the estimated product composition (see also <b>PRMN</b> ).																						
	Reactor Models	<ul style="list-style-type: none"><li>• Diffusion or Premixed Opposed-flow Flame</li><li>• Premixed Laminar Burner-stabilized Flame</li><li>• Premixed Laminar Flame-speed Calculation</li><li>• Rotating Disk CVD Reactor</li><li>• Stagnation Flow CVD Reactor</li></ul>																						
	Notes	<ul style="list-style-type: none"><li>• Any given species may simultaneously be included as a reactant (<b>REAC</b>), intermediate (<b>INTM</b>), and product (<b>PROD2</b>).</li><li>• The <b>PROD2</b> keywords must be changed as a set, not individually for a restart run.</li><li>• The <b>PROD2</b> keywords must be changed as a set, not individually for continuation run.</li></ul>																						
<b>PROE</b>  Reactor Property	<p>Assigns the initial (or estimate for steady-state calculations) number density of the particle consisting of the designated material name. The default value is 0. The reactor number is optional. When no reactor number is given, the same initial particle mass density will apply to all reactors in the network. The <b>PROE</b> keyword must be used in conjunction with the <b>PNDE</b> keyword and is mutually exclusive to keyword <b>PVFE</b>. When both <b>PNDE</b> and <b>PROE</b> are given, the moments are calculated as</p> $M_0 = \text{PNDE}$ $M_1 = \frac{\text{PROE}}{m_0}$ $M_i = (\Delta C_{\text{nuc1}}) \times M_{i-1} \quad 1 < i \leq \text{NMOM}$ <p>where <math>m_0</math> is the mass of a material name molecule and <math>\rho_B</math> is the mass density of the bulk material.</p> <table><tr><th>Parameters</th><th>Optional/Reqd.</th><th>Units</th><th>Examples</th></tr><tr><td>Material name</td><td>Required</td><td>--</td><td>PROE <b>C(B)</b> 1.0E-10 1</td></tr><tr><td>Mass density</td><td>Required</td><td>gm/cm<sup>3</sup></td><td>PROE C(B) <b>1.0E-10</b> 1</td></tr><tr><td>Reactor number</td><td>Optional</td><td>--</td><td>PROE C(B) 1.0E-10 <b>1</b></td></tr><tr><td>Keyword Usage</td><td colspan="3">Optional keyword. The default value for the mass density is 0. <b>PNDE</b> keyword required. Cannot be used with <b>PVFE</b>.</td></tr></table>				Parameters	Optional/Reqd.	Units	Examples	Material name	Required	--	PROE <b>C(B)</b> 1.0E-10 1	Mass density	Required	gm/cm <sup>3</sup>	PROE C(B) <b>1.0E-10</b> 1	Reactor number	Optional	--	PROE C(B) 1.0E-10 <b>1</b>	Keyword Usage	Optional keyword. The default value for the mass density is 0. <b>PNDE</b> keyword required. Cannot be used with <b>PVFE</b> .		
Parameters	Optional/Reqd.	Units	Examples																					
Material name	Required	--	PROE <b>C(B)</b> 1.0E-10 1																					
Mass density	Required	gm/cm <sup>3</sup>	PROE C(B) <b>1.0E-10</b> 1																					
Reactor number	Optional	--	PROE C(B) 1.0E-10 <b>1</b>																					
Keyword Usage	Optional keyword. The default value for the mass density is 0. <b>PNDE</b> keyword required. Cannot be used with <b>PVFE</b> .																							

Keyword	Definition			
	<b>Reactor Models</b>	<ul style="list-style-type: none"><li>• Closed Homogeneous Batch Reactor</li><li>• Closed Plasma Reactor</li><li>• Cylindrical Shear Flow Reactor</li><li>• Honeycomb Monolith Reactor</li><li>• IC HCCI Engine</li><li>• Perfectly Stirred Reactor (PSR)</li><li>• Planar Shear Flow Reactor</li><li>• Plasma PSR</li><li>• Plasma Plug Flow Reactor</li><li>• Plug Flow Reactor</li><li>• SI Engine Zonal Simulator</li></ul>		
<b>PROI</b>  Inlet Property	Assigns the mass density of the particle consisting of the designated material name to the named inlet stream. The default value is 0. The stream name is optional if there is only one inlet. The PROI keyword must be used in conjunction with the <a href="#">PNDI</a> keyword and is mutually exclusive to keyword <a href="#">PVFI</a> .			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Stream name</i>	<b>Optional if there is only one inlet.</b>	--	PROI <b>EGR</b> C(B) 1.0E-10
	<i>Material name</i>	Required	--	PROI EGR <b>C(B)</b> 1.0E-10
	<i>Number density</i>	Required	gm/cm <sup>3</sup>	PROI EGR C(B) <b>1.0E-10</b>
	<b>Keyword Usage</b>	Optional keyword. Must be used with <a href="#">PNDI</a> . Cannot be used with <a href="#">PVFI</a> . The default value for the number density is 0.		
	<b>Reactor Models</b>	<ul style="list-style-type: none"><li>• Cylindrical Shear Flow Reactor</li><li>• Honeycomb Monolith Reactor</li><li>• Perfectly-stirred Reactor (PSR)</li><li>• Planar Shear Flow Reactor</li><li>• Plasma PSR</li><li>• Plasma Plug Flow Reactor</li><li>• Plug-flow Reactor (PFR)</li></ul>		

Keyword	Definition			
PS  Problem Type	Constant pressure and entropy constraints.			
	Keyword Usage	Optional keyword. Exactly one problem-type keyword must be included.		
	Reactor Models	• Chemical and Phase Equilibrium Calculations		
	Notes	• <a href="#">SP</a> keyword.is equivalent.		
PS-BAR  Reactor Property	The piston head area to bore area ratio.			
	Parameters	Optional/Reqd.	Units	Examples
	Ratio of piston head area to bore area.	Required	None	PSBAR <b>1.1</b>
	Keyword Usage	Optional keyword. Default = 1.0.		
	Reactor Models	• IC HCCI Engine  • Multi-zone HCCI Engine  • SI Engine Zonal Simulator		
	Notes	PSBAR should be > 1.0.		
PSURF  Inlet Property	Initial surface coverage on particles by the surface site species in the inlet flow.			
	Parameters	Optional/Reqd.	Units	Examples
	Stream name	<b>Optional if there is only one inlet.</b>	--	PSURF <b>inlet1</b> C(S) 0.1
	Surface species name	Required	--	PSURF inlet1 <b>C(S)</b> 0.1
	Surface coverage	Required	--	PSURF inlet1 C(S) <b>0.1</b>
	Keyword Usage	Optional keyword		
	Reactor Models	• Honeycomb Reactor  • Opposed-flow Flame  • Perfectly Stirred Reactor (PSR)  • Plasma Plug Flow Reactor  • Plasma PSR  • Plug Flow Reactor  • Premixed Laminar Burner-stabilized Flame  • Premixed Laminar Flame-speed Calculation		



Keyword	Definition			
PSV  Solver	Pseudo-velocity for use in modifying the surface species equations for improved convergence. This pseudo-convection term is incorporated into the surface site fraction equations in order to convert algebraic equations to differential equations. The value of the <b>PSV</b> should be small enough such that it has no effect on the solution results, but large enough to affect the convergence behavior. If not supplied, then the unmodified equations are used. The modified equations are sometimes helpful in reaching steady-state conditions for problems with stiff surface chemistry (e.g. catalytic combustion), but should not be used if no convergence problems are encountered. A recommended value to try for <b>PSV</b> would be about 1/10th of the inlet velocity, but the simulation should be repeated with smaller or larger values to make sure that it has no effect on the solution.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Pseudo-velocity</i>	Required	cm/sec	PSV <b>10</b> .
	<b>Keyword Usage</b>	Optional keyword. By default, the value is set to 10* <b>ATOL</b> .		
	<b>Reactor Models</b>	<ul style="list-style-type: none"><li>• Honeycomb Reactor</li><li>• Plasma Plug Flow Reactor</li><li>• Plug Flow Reactor</li></ul>		
PTM_SECTION_NUM  Reactor Property	The number of sections to use for the specified material.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Material name</i>	Required	--	PTM_SECTION_NUM <b>SOOT 30</b>
	<i>Number of sections</i>	Required	--	PTM_SECTION_NUM <b>SOOT 30</b>
	<b>Keyword Usage</b>	Required when the Sectional Model is used.		
	<b>Reactor Models</b>	<ul style="list-style-type: none"><li>• Opposed-flow Flame</li><li>• Plug Flow Reactor</li><li>• Premixed Laminar Burner Stabilized Flame</li><li>• Premixed Laminar Burner Stabilized Stagnation Flame</li><li>• Premixed Laminar Flame Speed Calculator</li></ul>		
PTM_SECTION_SIZEDEP_A0  Reactor Property	Tanh function constant that is used to blend lower and upper bounds of collision efficiency.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Material name</i>	Required	None	PTM_SECTION_SIZEDEP_A0 <b>SOOT 5</b>
	<i>A0</i>	Required	None	PTM_SECTION_SIZEDEP_A0 <b>SOOT 5</b>
	<b>Keyword Usage</b>	Optional keyword. Default size is 7.		
	<b>Reactor Models</b>	<ul style="list-style-type: none"><li>• Closed Homogeneous Batch Reactor</li></ul>		

Keyword	Definition			
		<ul style="list-style-type: none"><li>Internal Combustion Engine</li><li>Perfectly Stirred Reactor (PSR)</li><li>Diffusion or Premixed Opposed Flow Flame</li><li>Plug Flow Reactor</li><li>Premixed Laminar Burner Stabilized Flame</li><li>Premixed Laminar Burner Stabilized Stagnation Flame</li><li>Premixed Laminar Flame Speed Calculator</li></ul>		
PTM_SECTION_SIZEDEP_COEFF	Use size-dependent collision efficiency for particles .			
Reactor Property	Parameters	Optional/Reqd.	Units	Examples
	Material name	Required	None	PTM_SECTION_SIZEDEP_COEFF SOOT
	Keyword Usage	Optional keyword. Not used by default.		
	Reactor Models	<ul style="list-style-type: none"><li>Closed Homogeneous Batch Reactor</li><li>Internal Combustion Engine</li><li>Perfectly Stirred Reactor (PSR)</li><li>Diffusion or Premixed Opposed Flow Flame</li><li>Plug Flow Reactor</li><li>Premixed Laminar Burner Stabilized Flame</li><li>Premixed Laminar Burner Stabilized Stagnation Flame</li><li>Premixed Laminar Flame Speed Calculator</li></ul>		
PTM_SECTION_SIZEDEP_DSTAR	Limit diameter for size-dependent collision efficiency.			
Reactor Property	Parameters	Optional/Reqd.	Units	Examples
	Material name	Required	None	PTM_SECTION_SIZEDEP_DSTAR SOOT 13-06
	Diameter	Required	None	PTM_SECTION_SIZEDEP_DSTAR SOOT 13-06
	Keyword Usage	Optional keyword. No default value is given and must be specified by user when using size-dependent collision efficiency. For soot simulation, the value generally ranges from 10 to 20 nm.		
	Reactor Models	<ul style="list-style-type: none"><li>Closed Homogeneous Batch Reactor</li><li>Internal Combustion Engine</li><li>Perfectly Stirred Reactor (PSR)</li></ul>		

Keyword	Definition			
		<ul style="list-style-type: none"><li>• Diffusion or Premixed Opposed Flow Flame</li><li>• Plug Flow Reactor</li><li>• Premixed Laminar Burner Stabilized Flame</li><li>• Premixed Laminar Burner Stabilized Stagnation Flame</li><li>• Premixed Laminar Flame Speed Calculator</li></ul>		
<b>PTM_SECTION_SIZEDEP_HAMAKER</b>  Reactor Property	Hamaker constant for computing potential well depth when using size-dependent dispersion efficiency for particles.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Material name</i>	Required	None	PTM_SECTION_SIZEDEP_HAMAKER <b>SOOT 5e-13</b>
	<i>Diameter</i>	Required	None	PTM_SECTION_SIZEDEP_HAMAKER <b>SOOT 5e-13</b>
	<b>Keyword Usage</b>	Optional keyword. Default value is 7e-13 erg.		
	<b>Reactor Models</b>	<ul style="list-style-type: none"><li>• Closed Homogeneous Batch Reactor</li><li>• Internal Combustion Engine</li><li>• Perfectly Stirred Reactor (PSR)</li><li>• Diffusion or Premixed Opposed Flow Flame</li><li>• Plug Flow Reactor</li><li>• Premixed Laminar Burner Stabilized Flame</li><li>• Premixed Laminar Burner Stabilized Stagnation Flame</li><li>• Premixed Laminar Flame Speed Calculator</li></ul>		
<b>PTM_SECTION_SNO</b>  Reactor Property	Number of “atoms” in the smallest section for the specified material. When etching reactions are present, the number of sectional atoms parameter needs to be unity. When only growth is present, the user can give some higher value to avoid calculations for smaller particles that will never be present. However, this value must not be greater than the number of atoms in the smallest nucleating particle.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Material name</i>	Required	--	PTM_SECTION_SNO <b>SOOT 1</b>
	<i>Number of sectional “atoms”</i>	Required	--	PTM_SECTION_SNO <b>SOOT 1</b>
	<b>Keyword Usage</b>	Required when the Sectional Model is used.		
	<b>Reactor Models</b>	<ul style="list-style-type: none"><li>• Opposed-flow Flame</li><li>• Plug Flow Reactor</li></ul>		

Keyword	Definition			
		<ul style="list-style-type: none"><li>• Premixed Laminar Burner Stabilized Flame</li><li>• Premixed Laminar Burner Stabilized Stagnation Flame</li><li>• Premixed Laminar Flame Speed Calculator</li></ul>		
PTM_SECTION_SPACING  Reactor Property	Geometric spacing factor to be used for sections.			
	Parameters	Optional/Reqd.	Units	Examples
	Material name	Required	--	PTM_SECTION_SPACING <b>CARBON 2.0</b>
	Geometric spacing factor	Required	--	PTM_SECTION_SPACING <b>CARBON 2.0</b>
	Keyword Usage	Required when the Sectional Model is used.		
	Reactor Models	<ul style="list-style-type: none"><li>• Opposed-flow Flame</li><li>• Plug Flow Reactor</li><li>• Premixed Laminar Burner Stabilized Flame</li><li>• Premixed Laminar Burner Stabilized Stagnation Flame</li><li>• Premixed Laminar Flame Speed Calculator</li></ul>		
PTM_SECTION_TCOND  Reactor Property	Thermal conductivity of particle material. This is a required input when any of the flame models are using the Sectional Model with thermophoresis.			
	Parameters	Optional/Reqd.	Units	Examples
	Material name	Required	--	PTM_SECTION_TCOND <b>CARBON 2.0E+05</b>
	Thermal conductivity of "material"	Required	erg/s-cm-K	PTM_SECTION_TCOND <b>CARBON 2.0E+05</b>
	Keyword Usage	Required when the Sectional Model with thermophoresis is used.		
	Reactor Models	<ul style="list-style-type: none"><li>• Opposed-flow Flame</li><li>• Plug Flow Reactor</li><li>• Premixed Laminar Burner Stabilized Flame</li><li>• Premixed Laminar Burner Stabilized Stagnation Flame</li><li>• Premixed Laminar Flame Speed Calculator</li></ul>		
PTM_SECTION_USER_BULK-PROP	User-specified enhancement factor for the growth/etching reactions on particles. This can be used only with the sectional method. Note that the user-routines library must be compiled and linked; see the Chemkin-Pro Application Programming Interface Manual for details.			

Keyword	Definition			
Reactor Property	Parameters	Optional/Reqd.	Units	Examples
	<i>Material name</i>	Required	None	PTM_SECTION_USERBULKROP <b>CARBON</b>
	<b>Keyword Usage</b>	Optional keyword. Not used by default.		
	<b>Reactor Models</b>	<ul style="list-style-type: none"><li>• Closed Homogeneous Batch Reactor</li><li>• IC HCCI Engine</li><li>• Multi-Zone HCCI Engine Simulator</li><li>• SI Engine Zonal Simulator</li><li>• Perfectly Stirred Reactor (PSR)</li><li>• Plug Flow Reactor</li><li>• Opposed-flow Flame</li><li>• Premixed Laminar Burner Stabilized Flame</li><li>• Premixed Laminar Burner Stabilized Stagnation Flame</li><li>• Premixed Laminar Flame Speed Calculator</li></ul>		
<b>PTM_SECTION-AL</b>  Reactor Property	Signals that sectional model is to be used. This is a required keyword when the Sectional Model is used.			
	<b>Keyword Usage</b>	Required when the Sectional Model is used.		
	<b>Reactor Models</b>	<ul style="list-style-type: none"><li>• Closed Homogeneous Batch Reactor</li><li>• IC HCCI Engine</li><li>• Multi-Zone HCCI Engine Simulator</li><li>• SI Engine Zonal Simulator</li><li>• Perfectly Stirred Reactor (PSR)</li><li>• Opposed-flow Flame</li><li>• Plug Flow Reactor</li><li>• Premixed Laminar Burner Stabilized Flame</li><li>• Premixed Laminar Burner Stabilized Stagnation Flame</li><li>• Premixed Laminar Flame Speed Calculator</li></ul>		
<b>PV</b>  Problem Type	Constant pressure and volume constraints.			
	<b>Keyword Usage</b>	Optional keyword. Exactly one problem-type keyword must be included.		
	<b>Reactor Models</b>	<ul style="list-style-type: none"><li>• Chemical and Phase Equilibrium Calculations</li></ul>		

Keyword	Definition																		
	Notes	• <b>VP</b> keyword is equivalent.																	
<b>PVFE</b>  Reactor Property	<p>Assigns the initial (or estimate for steady state calculations) number density of the particle consisting of the designated material name. The default value is 0. The reactor number is optional. When no reactor number is given, the same initial particle volume fraction will apply to all reactors in the network. The PVFE keyword must be used in conjunction with the <b>PNDE</b> keyword and is mutually exclusive to keyword <b>PROE</b>. When both PNDE and PVFE are given, the moments are calculated as</p> $M_0 = \text{PNDE}$ $M_1 = \frac{\rho_B \times \text{PVFE}}{m_0}$ $M_i = (\Delta C_{\text{nuc1}}) \times M_{i-1} \quad 1 < i \leq \text{NMOM}$ <p>where <math>m_0</math> is the mass of a material name molecule and <math>\rho_B</math> is the mass density of the bulk material.</p> <table><tr><th>Parameters</th><th>Optional/Reqd.</th><th>Units</th><th>Examples</th></tr><tr><td>Material name</td><td>Required</td><td>--</td><td>PVFE <b>C(B)</b> 1.0E-10 4</td></tr><tr><td>Volume fraction</td><td>Required</td><td>cm<sup>3</sup> /cm<sup>3</sup></td><td>PVFE C(B) <b>1.0E-10</b> 4</td></tr><tr><td>Reactor number</td><td>Optional</td><td>--</td><td>PVFE C(B) 1.0E-10 <b>4</b></td></tr></table> <p><b>Keyword Usage</b></p> <p>Optional keyword. The default value is value for the volume fraction is 0. PNDE keyword required.</p> <p><b>Reactor Models</b></p> <ul style="list-style-type: none"><li>• Closed Homogeneous Batch Reactor</li><li>• Closed Plasma Reactor</li><li>• Cylindrical Shear Flow Reactor</li><li>• Honeycomb Monolith Reactor</li><li>• IC HCCI Engine</li><li>• Perfectly Stirred Reactor (PSR)</li><li>• Planar Shear Flow Reactor</li><li>• Plasma PSR</li><li>• Plasma Plug Flow Reactor</li><li>• Plug Flow Reactor</li><li>• SI Engine Zonal Simulator</li></ul>			Parameters	Optional/Reqd.	Units	Examples	Material name	Required	--	PVFE <b>C(B)</b> 1.0E-10 4	Volume fraction	Required	cm <sup>3</sup> /cm <sup>3</sup>	PVFE C(B) <b>1.0E-10</b> 4	Reactor number	Optional	--	PVFE C(B) 1.0E-10 <b>4</b>
Parameters	Optional/Reqd.	Units	Examples																
Material name	Required	--	PVFE <b>C(B)</b> 1.0E-10 4																
Volume fraction	Required	cm <sup>3</sup> /cm <sup>3</sup>	PVFE C(B) <b>1.0E-10</b> 4																
Reactor number	Optional	--	PVFE C(B) 1.0E-10 <b>4</b>																
<b>PVFI</b>	Assigns the volume fraction of the particle consisting of the designated material name to the named inlet stream. The default value is 0. The stream name is																		

Keyword	Definition			
Inlet Property	optional if there is only one inlet. The PVFI keyword must be used in conjunction with the <b>PNDI</b> keyword and is mutually exclusive to keyword <b>PROI</b> .			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Stream name</i>	<b>Optional if there is only one inlet.</b>	--	PVFI <b>mixture1</b> C(B) 1.0E--9
	<i>Material name</i>	Required	--	PVFI mixture1 <b>C(B)</b> 1.0E-9
	<i>Number density</i>	Required	cm <sup>3</sup> /cm <sup>3</sup>	PVFI mixture1 C(B) <b>1.0E-9</b>
	<b>Keyword Usage</b>	Optional keyword. Must be used with PNDI. Cannot be used with PROI. The default value for the number density is 0.		
	<b>Reactor Models</b>	<ul style="list-style-type: none"><li>• Cylindrical Shear Flow Reactor</li><li>• Honeycomb Monolith Reactor</li><li>• Perfectly-stirred Reactor (PSR)</li><li>• Planar Shear Flow Reactor</li><li>• Plasma PSR</li><li>• Plasma Plug Flow Reactor</li><li>• Plug-flow Reactor (PFR)</li></ul>		
PVS0 Reactor Property	Specify the reference gas viscosity at the reference temperature of the power-law for viscosity.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Reference gas viscosity at reference temperature</i>	Required.	g/cm-s	PVS0 <b>1.716E-4</b>
	<b>Keyword Usage</b>	Optional.		
	<b>Reactor Models</b>	<ul style="list-style-type: none"><li>• Multi-Zone HCCI Simulator</li><li>• IC HCCI Engine</li><li>• SI Engine Zonal Simulator</li></ul>		
PVSN Reactor Property	Specify the exponent of the temperature ratio term of the power-law for viscosity.			
	Parameters	Optional/Reqd.	Units	Examples

Keyword	Definition			
	<i>Exponent of temperature ratio term</i>	Required.	--	PVSN <b>0.5</b>
	<b>Keyword Usage</b>	Optional.		
	<b>Reactor Models</b>	<ul style="list-style-type: none"><li>Multi-Zone HCCI Simulator</li><li>IC HCCI Engine</li><li>SI Engine Zonal Simulator</li></ul>		
<b>PVST</b>	Specify the reference temperature of the power-law for viscosity.			
Reactor Property	Parameters	Optional/Reqd.	Units	Examples
	<i>Reference temperature</i>	Required.	K	PVST <b>273.15</b>
	<b>Keyword Usage</b>	Optional.		
	<b>Reactor Models</b>	<ul style="list-style-type: none"><li>Multi-Zone HCCI Simulator</li><li>IC HCCI Engine</li><li>SI Engine Zonal Simulator</li></ul>		
<b>PWRC</b>	The power being supplied to heat the deposition surface or disk. This value is used only if the disk temperature is being calculated from an energy balance by including keyword <b>RADB</b> . See <a href="#">Equation 14.18</a> of the <a href="#">Chemkin-Pro Theory Manual</a> .			
Reactor Property	Parameters	Optional/Reqd.	Units	Examples
	<i>Power</i>	Required	cal/(cm <sup>2</sup> . sec)	PWRC <b>15.E7</b>
	<b>Keyword Usage</b>	Optional keyword. By default, the power is 0.0.		
	<b>Reactor Models</b>	<ul style="list-style-type: none"><li>Rotating Disk CVD Reactor</li><li>Stagnation Flow CVD Reactor</li></ul>		
<b>PWRW</b>	Total power deposition to the plasma.			
Reactor Property	Parameters	Optional/Reqd.	Units	Examples
	<i>Total power deposition</i>	Required	Watts	PWRW <b>1000.</b>
	<i>Reactor number (PSR clusters only)</i>	Optional  If no number is given, the value is assumed to apply	--	PWRW 1000. <b>1</b>



Keyword	Definition			
		to all reactors in a cluster.		
	Keyword Usage	Required keyword.		
	Reactor Models	<ul style="list-style-type: none"><li>• Closed Plasma Reactor</li><li>• Plasma Plug Flow Reactor</li><li>• Plasma PSR</li></ul>		
QDOT Reactor Property	The power being supplied to heat the gas as a spatially distributed Gaussian heat source. QDOT is the total power, i.e., the spatial integral of the heat source function. See Equation 14.14 of the Chemkin-Pro Theory Manual .			
	Parameters	Optional/Reqd.	Units	Examples
	Power	Required	erg/(cm <sup>2</sup> . sec)	QDOT 1.0E7
	Keyword Usage	Optional keyword. By default, the power is 0.0.		
	Reactor Models	<ul style="list-style-type: none"><li>• Rotating Disk CVD Reactor</li><li>• Stagnation Flow CVD Reactor</li></ul>		
QDTC Reactor Property	The power being supplied to heat the gas as a spatially distributed Gaussian heat source. QDTC is the total power, i.e., the spatial integral of the heat source function. See Equation 14.14 of the Chemkin-Pro Theory Manual .			
	Parameters	Optional/Reqd.	Units	Examples
	Power	Required	cal/(cm <sup>2</sup> . sec)	QDTC 1.0E7
	Keyword Usage	Optional keyword. By default, the power is 0.0.		
	Reactor Models	<ul style="list-style-type: none"><li>• Rotating Disk CVD Reactor</li><li>• Stagnation Flow CVD Reactor</li></ul>		
QEXP Reactor Property	Specifies the gas chemistry heat release rate that defines the start of the expansion period. This keyword will take effect only when the gas heat release equation is solved (activated by keyword: QRGEQ ).			
	Parameters	Optional/Reqd.	Units	Examples
	heat_release_rate	Required	cal/sec	QEXP 0.5
	Keyword Usage	Optional keyword. Default is 0.1 cal/sec.		
	Reactor Models	<ul style="list-style-type: none"><li>• Multi-Zone HCCI Simulator</li><li>• IC HCCI Engine</li><li>• SI Engine Zonal Simulator</li></ul>		

Keyword	Definition			
QFUN  Reactor Property User Subroutine	Reactor heat loss will be given as a specified function of time (for 0-D homogeneous reactors) or as a function of distance (for Plug Flow Reactors), through a user-programmed subroutine. FUNCTION PSQFUN (LENIQ, LENRQ, IQFUN, RQFUN) must be provided to specify the heat loss and linked to the application program. See the Application Programming Interface Manual for details on how to work with user subroutines.			
	Keyword Usage	Optional keyword. By default, the value there is no heat loss from the reactor. The units returned from the user subroutine must be in erg/sec. See also QPRO.		
	Reactor Models	<ul style="list-style-type: none"><li>• Closed Homogeneous Batch Reactor</li><li>• Closed Plasma Reactor</li><li>• Diffusion or Premixed Opposed-flow Flame</li><li>• Honeycomb Reactor</li><li>• IC HCCI Engine</li><li>• Non-reactive Gas Mixer</li><li>• Perfectly Stirred Reactor (PSR)</li><li>• Plasma Plug Flow Reactor</li><li>• Plasma PSR</li><li>• Plug Flow Reactor</li><li>• Premixed Laminar Burner-stabilized Flame</li><li>• Premixed Laminar Flame-speed Calculation</li><li>• SI Engine Zonal Simulator</li></ul>		
	Notes	<ul style="list-style-type: none"><li>• See also QPRO as an alternate way to specify heat-loss as a function of time.</li><li>• Keywords QFUN, QLOS and QPRO are mutually exclusive.</li></ul>		
QIAGE  Reactor Property/Model	The time delay to turn on the droplet temperature equation at the beginning of liquid vaporization to prevent possible convergence issues at the start of injection. When the <b>Droplet Surface T = Core T</b> option is selected, a very large time delay can force the droplet temperature to be constant, that is, equal to the initial liquid temperature, throughout the simulation.			
	Parameters	Optional/Reqd.	Units	Examples
	Time	Required	seconds	QIAGE 1.0E-3
	Keyword Usage	Optional keyword. Default is 0.0 sec.		
	Reactor Models	<ul style="list-style-type: none"><li>• Direct Injection Diesel Engine Simulator</li></ul>		

Keyword	Definition			
QLOS  Reactor Property	The heat loss or heat flux from the reactor to the external environment at an optionally specified surface material. The units are for a total heat loss for 0-D homogeneous reactors, or for heat flux per area for all channel-flow reactors (Plug Flow Reactor, Honeycomb Reactor, Plasma Plug Flow Reactor, and Shear Flow Reactors). This option is only relevant when the energy equation is being solved.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Material name (for 0-D homogeneous and plug-flow reactors only)</i>	Optional  If no material is specified, the value will be used for all materials.	--	QLOS <b>material1</b> 50
	<i>Heat loss or Heat flux (depending on Reactor Model)</i>	Required	cal/sec or cal/cm2-s	QLOS 50
	<i>Reactor number (PSR clusters only)</i>	Optional  If no number is given, the keyword is assumed to apply to all reactors in a cluster.	--	QLOS material1 50 <b>1</b>
	<b>Keyword Usage</b>	Optional keyword. By default, there is no heat loss from the reactor. See also <a href="#">QPRO</a> , <a href="#">HTRN</a> , and <a href="#">QFUN</a> .		
	<b>Reactor Models</b>	<ul style="list-style-type: none"> <li>• Closed Homogeneous Batch Reactor</li> <li>• Closed Plasma Reactor</li> <li>• Cylindrical Shear Flow Reactor</li> <li>• Honeycomb Reactor</li> <li>• IC HCCI Engine</li> <li>• Non-reactive Gas Mixer</li> <li>• Planar Shear Flow Reactor</li> </ul>		

Keyword	Definition			
		<ul style="list-style-type: none"><li>• Plasma Plug Flow Reactor</li><li>• Plug Flow Reactor</li><li>• Perfectly Stirred Reactor (PSR)</li><li>• SI Engine Zonal Simulator</li></ul>		
<b>QLSE</b>  Reactor Property Profiles	This is an additional energy loss term for the electrons that may be introduced to account for inelastic collisional losses that are not already included explicitly in the <i>Gas-phase Kinetics</i> reaction mechanism. Energy loss values are specified here as a function of electron temperature and are given per ionization event to be consistent with the work of Lee, et al.[11] (p. 345) For example, "QLSE 34800. 100." would represent an electron energy loss of 100 eV/ionization event for an electron temperature of 34800 K (3.0 eV).			
	Parameters	Optional/Reqd.	Units	Examples
	Energy loss	Required	eV	QLSE <b>34800.</b> 100.
	Electron temperature	Required	K	QLSE 34800. <b>100.</b>
	<b>Keyword Usage</b>	Optional keyword. By default, the additional energy loss term is 0.0.		
	<b>Reactor Models</b>	<ul style="list-style-type: none"><li>• Closed Plasma Reactor</li><li>• Plasma Plug Flow Reactor</li><li>• Plasma PSR</li></ul>		
<b>QPRO</b>  Reactor Property Profiles	The heat loss profile or heat flux profile from the reactor to the external environment at an optionally specified surface material, given as a piece-wise linear function of time or distance. Each <b>QPRO</b> entry represents a point in a piecewise-linear profile. The units are for a total heat loss vs. time for 0-D homogeneous reactors, or for heat flux per area vs. distance for all channel-flow reactors (Plug Flow Reactor, Honeycomb Reactor, Plasma Plug Flow Reactor, and Shear Flow Reactors). This option is only relevant when the energy equation is being solved.			
	Parameters	Optional/Reqd.	Units	Examples
	Time or Distance value (depending on Reactor Model)	Required	sec or cm	QPRO <b>1.0E-4</b> 10.0
	Heat loss or Heat flux (depending on Reactor Model)	Required	cal/sec or cal/cm2-sec	QPRO 1.0E-4 <b>10.0</b>
	Reactor number (PSR clusters only)	Optional	--	QPRO 1.0E-4 10.0 <b>1</b>
		If no number is given, the		

Keyword	Definition			
		profile described by the first two values is assumed to apply to all reactors in a cluster.		
	Keyword Usage	Optional keyword. By default, there is no heat loss from the reactor. See also <a href="#">QLOS</a> , <a href="#">HTRN</a> , and <a href="#">QFUN</a> .		
	Reactor Models	<ul style="list-style-type: none"><li>• Closed Homogeneous Batch Reactor</li><li>• Closed Plasma Reactor</li><li>• Cylindrical Shear Flow Reactor</li><li>• Honeycomb Reactor</li><li>• IC HCCI Engine</li><li>• Non-reactive Gas Mixer</li><li>• Perfectly Stirred Reactor (PSR)</li><li>• Planar Shear Flow Reactor</li><li>• Plasma PSR</li><li>• Plasma Plug Flow Reactor</li><li>• Plug Flow Reactor</li><li>• SI Engine Zonal Simulator</li></ul>		
QRGEQ Output	Solve a separate equation that integrates the heat release due to gas-phase reactions to obtain a more accurate heat-release profile. If this option is not checked, only local heat release rates will be reported at each saved or printed time steps. Only applicable when you are solving the energy equation with transient solver.			
	Parameters	Optional/Reqd.	Units	Examples
	Keyword Usage	Optional keyword. By default, the heat release integration equation is not solved.		
	Reactor Models	<ul style="list-style-type: none"><li>• Closed Homogeneous Batch Reactor</li><li>• Closed Plasma Reactor</li><li>• Honeycomb Monolith Reactor</li></ul>		

Keyword	Definition			
		<ul style="list-style-type: none"><li>• IC HCCI Engine</li><li>• Perfectly Stirred Reactor (PSR)</li><li>• Plasma PSR</li><li>• Plasma Plug Flow Reactor</li><li>• Plug Flow Reactor</li><li>• SI Engine Zonal Simulator</li></ul>		
QRSEQ  Output	Solve a separate equation that integrates the heat release due to surface reactions to obtain a more accurate heat-release profile. If this option is not checked, only local heat release rates will be reported at each saved or printed time steps. Only applicable when you are solving the energy equation with transient solver.			
	Parameters	Optional/Reqd.	Units	Examples
	Keyword Usage	Optional keyword. By default, the heat release integration equation is not solved.		
	Reactor Models	<ul style="list-style-type: none"><li>• Closed Homogeneous Batch Reactor</li><li>• Closed Plasma Reactor</li><li>• Honeycomb Monolith Reactor</li><li>• IC HCCI Engine</li><li>• Perfectly Stirred Reactor (PSR)</li><li>• Plasma PSR</li><li>• Plasma Plug Flow Reactor</li><li>• Plug Flow Reactor</li></ul>		
QXCO  Recycling	This keyword defines the heat-transfer coefficient and the heat-transfer surface area for thermal conductive/convective heat flux between the two specified reactors in a reactor cluster. The direction of the heat flux will come from the higher-temperature reactor to the lower-temperature reactor. This keyword is only relevant when the ENRG keyword is used and when there are multiple reactors in a cluster.			
	Parameters	Optional/Reqd.	Units	Examples
	Reactor Number	Required	--	QXCO 3 6 1.0E-3 1000.
	Reactor Number	Required	--	QXCO 3 6 1.0E-3 1000.
	Heat-transfer coefficient	Required	cal/(cm <sup>2</sup> · sec · K)	QXCO 3 6 1.0E-3 1000.
	Heat-transfer surface area	Required	cm <sup>2</sup>	QXCO 3 6 1.0E-3 1000.

Keyword	Definition			
	<b>Keyword Usage</b>	Optional keyword. By default, there is no heat exchange between reactors.		
	<b>Reactor Models</b>	<ul style="list-style-type: none"><li>Perfectly Stirred Reactor (PSR)</li><li>Plasma PSR</li></ul>		
	<b>Notes</b>	<ul style="list-style-type: none"><li>The order of the two reactor numbers that define the heat connection is not important.</li><li>This parameter is used in conjunction with the external surface area (<a href="#">AREAQ</a> or <a href="#">AEXT</a>).</li></ul>		
<b>QXRA</b> Recycling	This keyword defines the thermal emissivity/absorptivity and the heat-transfer surface area for thermal radiative flux between the two specified reactors in a reactor cluster. The direction of the heat flux will come from the higher-temperature reactor to the lower-temperature reactor. This keyword is only relevant when the <a href="#">ENRG</a> keyword is used and when there are more than one reactor in a cluster.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Reactor Number</i>	Required	--	QXRA <b>2</b> 3 0.1 1000.
	<i>Reactor Number</i>	Required	--	QXRA 2 <b>3</b> 0.1 1000.
	<i>Emissivity/absorptivity</i>	Required	--	QXRA 2 3 <b>0.1</b> 1000.
	<i>Heat-transfer surface area</i>	Required	cm <sup>2</sup>	QXRA 2 3 0.1 <b>1000</b> .
	<b>Keyword Usage</b>	Optional keyword. By default, there is no heat exchange between reactors. Note that the order of the two reactor numbers that define the heat connection is un-important.		
	<b>Reactor Models</b>	<ul style="list-style-type: none"><li>Perfectly Stirred Reactor (PSR)</li><li>Plasma PSR</li></ul>		
	<b>Notes</b>	<ul style="list-style-type: none"><li>The order of the two reactor numbers that define the heat connection is not important.</li><li>This parameter is used in conjunction with the external surface area (<a href="#">AREAQ</a> or <a href="#">AEXT</a>).</li></ul>		
<b>RACTV</b> Reactor Property	By default, when the gas-phase thermal radiation calculation is on, contributions from all major radiating species (such as CO <sub>2</sub> , H <sub>2</sub> O, CO, and CH <sub>4</sub> ) will not be included. A major radiating species is a species of which the absorption coefficient is available to the application. This keyword allows the user to include the contribution of a major species in the radiation heat loss calculation.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Species symbol</i>	Required	--	RACTV CO
	<b>Keyword Usage</b>	Optional keyword.		
	<b>Reactor Models</b>	<ul style="list-style-type: none"><li>Diffusion or Premixed Opposed-flow Flame</li></ul>		

Keyword	Definition			
		<ul style="list-style-type: none"><li>• Burner-stabilized Pre-mixed Flame</li><li>• Premixed Laminar Flame-speed Calculation</li></ul>		
RADB  Reactor Property	Use an energy balance to determine the disk or susceptor (deposition surface) temperature. If RADB is specified, TDSK is used as the initial guess for the susceptor temperature.			
	Keyword Usage	Optional keyword. By default, the susceptor temperature is fixed as TDSK.		
	Reactor Models	<ul style="list-style-type: none"><li>• Rotating Disk CVD Reactor</li><li>• Stagnation Flow CVD Reactor</li></ul>		
RADGS  Reactor Property	Turns on the radiation heat loss term in the gas energy equation. The optional model number indicates which thermal radiation model will be employed to calculate the radiation intensity.			
	Parameters	Optional/Reqd.	Units	Examples
	Reactor number	Required	--	RADGS 0
	Keyword Usage	Currently, the optically-thin limit model is the only model implemented and hence is the default model. The model number for the optically-thin limit model is 0.		
	Reactor Models	<ul style="list-style-type: none"><li>• Diffusion or Premixed Opposed-flow Flame</li><li>• Burner-stabilized Pre-mixed Flame</li><li>• Premixed Laminar Flame-speed Calculation</li></ul>		
RADPT  Reactor Property	Allows radiative heat loss contribution from particulates associated with the named material to be included independently.			
	Parameters	Optional/Reqd.	Units	Examples
	Material Name	Required	--	RADPT CO
	Reactor Models	<ul style="list-style-type: none"><li>• Diffusion or Premixed Opposed-flow Flame</li><li>• Burner-stabilized Pre-mixed Flame</li><li>• Premixed Laminar Flame-speed Calculation</li></ul>		
RCHG  Solver	Maximum relative change in the surface site fractions (over one time step) for which the initial fictitious transient equations that establish the initial surface site fractions can be considered to have converged to steady state.			
	Parameters	Optional/Reqd.	Units	Examples
	Maximum relative change	Required	--	RCHG 1.0E-3
	Keyword Usage	Optional keyword. By default, the maximum relative change is set to 1.0E-6.		
	Reactor Models	<ul style="list-style-type: none"><li>• Honeycomb Reactor</li></ul>		



Keyword	Definition			
		<ul style="list-style-type: none"><li>• Plasma Plug Flow Reactor</li><li>• Plug Flow Reactor</li></ul>		
<b>RDSK</b>  Reactor Property	Ratio of the substrate radius to the separation distance between it and the upper radiating disk. This is used in calculating a surface radiation balance. <b>RRAD</b> is used only if the disk temperature is being calculated by including keyword <b>RADB</b> . See <a href="#">Equation 14.18</a> of the <a href="#">Chemkin-Pro Theory Manual</a> .			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Ratio of substrate</i>	Required	--	RDSK <b>3.0</b>
	<b>Keyword Usage</b>	Optional keyword. This is keyword is required only when <b>RRAD</b> and <b>RADB</b> are included.		
	<b>Reactor Models</b>	<ul style="list-style-type: none"><li>• Rotating Disk CVD Reactor</li><li>• Stagnation Flow CVD Reactor</li></ul>		
<b>REAC</b>  Inlet or Reactor Property	Mole fraction of the reagent gases entering the reactor for an inlet stream or for the initial conditions in a closed system. For example, REAC fuel1 C2H2 0.5, would indicate that acetylene has a mole fraction of 0.5 in the inlet stream named fuel1. The sum of all the reactant mole fractions should equal to one. However, if they do not the fractions will be normalized so that they do sum to one, and a warning message will be printed to the output file.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Inlet stream name (for PSRs and CVD Reactors only)</i>	Optional  If there is no stream name than the reactant and mole fraction apply to all streams.	--	REAC <b>fuel1</b> C2H2 0.5
	<i>Species name</i>	Required	--	REAC <b>C2H2</b> 0.5
	<i>Reactant fraction</i>	Required	mole fractions	REAC C2H2 <b>0.5</b>
	<b>Keyword Usage</b>	Required keyword, except in cases where an equivalence ratio option is used ( <a href="#">EQUI</a> ).		
	<b>Reactor Models</b>	<ul style="list-style-type: none"><li>• Chemical and Phase Equilibrium Calculations</li><li>• Closed Homogeneous Batch Reactor</li><li>• Closed Plasma Reactor</li><li>• Cylindrical Shear Flow Reactor</li></ul>		

Keyword	Definition			
	<ul style="list-style-type: none"> <li>• Diffusion or Premixed Opposed-flow Flame</li> <li>• Honeycomb Reactor</li> <li>• IC HCCI Engine</li> <li>• Non-reactive Gas Mixer</li> <li>• Partially Stirred Reactor (PaSR)</li> <li>• Perfectly Stirred Reactor (PSR)</li> <li>• Planar Shear Flow Reactor</li> <li>• Plasma Plug Flow Reactor</li> <li>• Plasma PSR</li> <li>• Plug Flow Reactor</li> <li>• Premixed Laminar Burner-stabilized Flame</li> <li>• Premixed Laminar Flame-speed Calculation</li> <li>• Rotating Disk CVD Reactor</li> <li>• Stagnation Flow CVD Reactor</li> </ul>			
	<b>Notes</b> <ul style="list-style-type: none"> <li>• The <b>REAC</b> keywords must be changed as a set, not individually for a restart run.</li> <li>• The <b>REAC</b> keywords must be changed as a set, not individually for continuation run.</li> </ul>			
<b>RECY</b>	For a cluster of reactors ( $NPSR > 1$ ), specifies recycling or routing of a mass flow from one reactor to another and the fractional flow associated with this stream.			
Recycling	Parameters	Optional/Reqd.	Units	Examples
	Reactor Number, from which the flow originates	Required	--	RECY 2 1 0.3
	Reactor Number, to which the flow is transferred	Required	--	RECY 2 1 0.3
	Percent that will be recycled from Reactor 2 back into Reactor 1	Required	--	RECY 2 1 <b>0.3</b>
	<b>Keyword Usage</b>	Optional keyword. By default all flow out of a reactor in will flow into the next reactor in the series (e.g. RECY 1 2 1.0 and RECY 2 3 1.0 for a three-reactor system). If recycle loops are defined, then the effective "recycling"		

Keyword	Definition			
		from the upstream into the downstream reactor will be one minus the sum of the recycle streams out of the upstream reactor into other reactors.		
	Reactor Models	<ul style="list-style-type: none"><li>• Perfectly Stirred Reactor (PSR)</li><li>• Plasma PSR</li></ul>		
RE-LAXC Solver	Controls the convergence method used for transient runs. When applied, it uses a relaxed scheme whereby the integrator solver tries harder to achieve a solution at each time, but occasionally may result in increased time to solve your problem or numerical instabilities. Therefore, you should use this only if your transient run fails with a “nonlinear solver failed to converge repeatedly” message or you believe your problem is very stiff, highly nonlinear or discontinuous.			
	Keyword Usage	Optional keyword.		
	Reactor Models	<ul style="list-style-type: none"><li>• Closed Homogeneous Batch Reactor</li><li>• Closed Partially Stirred Reactor</li><li>• Closed Plasma Reactor</li><li>• Cylindrical Shear Flow Reactor</li><li>• Honeycomb Reactor</li><li>• IC HCCI Engine</li><li>• Multi-Zone HCCI Engine Simulator</li><li>• Partially Stirred Reactor (PaSR)</li><li>• Perfectly Stirred Reactor (PSR)</li><li>• Planar Shear Flow Reactor</li><li>• Plasma Plug Flow Reactor</li><li>• Plasma PSR</li><li>• Plug Flow Reactor</li><li>• Rotating Disk CVD Reactor</li><li>• SI Engine Zonal Simulator</li><li>• Stagnation Flow CVD Reactor</li></ul>		
RELT Solver	This keyword is used to override the default value for the relative perturbation in the solution variable used in the determination of the numerically derived Jacobian.			
	Parameters	Optional/Reqd.	Units	Examples

Keyword	Definition			
	<i>Relative perturbation</i>	Required	--	RELT <b>1.E-15</b>
	<b>Keyword Usage</b>	Optional keyword. By default, the relative perturbation is set equal to the square root of the unit round-off error of the machine.		
	<b>Reactor Models</b>	<ul style="list-style-type: none"><li>• Non-reactive Gas Mixer</li><li>• Perfectly Stirred Reactor (PSR)</li><li>• Plasma PSR</li></ul>		
<b>RE-OR</b>  Reactor Property	The option may be used when the <a href="#">TRCE</a> option is in effect. Using <a href="#">TRCE</a> , the conservation equation for the last species in the gas-phase and each surface and bulk phase is not solved: the last species concentration (mass fraction or site fraction) is chosen so that the fractions sum to one. The <a href="#">REOR</a> option causes <a href="#">TRCE</a> to choose dynamically and locally (at each mesh point and in each phase) the species of largest concentration and not solve its conservation equation.			
	<b>Keyword Usage</b>	Optional keyword. By default, the last species in each phase is chosen.		
	<b>Reactor Models</b>	<ul style="list-style-type: none"><li>• Rotating Disk CVD Reactor</li><li>• Stagnation Flow CVD Reactor</li></ul>		
<b>RHO1</b>  Reactor Property	Mass density before the incident shock.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Mass density</i>	Required	gm/cm <sub>3</sub>	RHO1 <b>1.E-4</b>
	<b>Keyword Usage</b>	Optional keyword. The shock velocity and any two of temperature, pressure, or density must be specified for conditions before the incident shock. See also <a href="#">T1</a> and <a href="#">P1A</a> .		
	<b>Reactor Models</b>	<ul style="list-style-type: none"><li>• Normal Incident Shock</li><li>• Normal Reflected Shock</li></ul>		
<b>RHO2</b>  Reactor Property	Mass density after the incident shock.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Mass density</i>	Required	g/cm <sub>3</sub>	RHO2 <b>1.E-4</b>
	<b>Keyword Usage</b>	Optional keyword. Any two of temperature, pressure, or density must be specified for conditions after the incident shock. See also <a href="#">T2</a> and <a href="#">P2A</a> .		
	<b>Reactor Models</b>	<ul style="list-style-type: none"><li>• Normal Incident Shock</li><li>• Normal Reflected Shock</li></ul>		

Keyword	Definition			
RHO3  Reactor Property	Mass density after the reflected shock.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Mass density</i>	Required	g/cm <sup>3</sup>	RHO3 <b>1.E-4</b>
	<b>Keyword Usage</b>	Optional keyword. Any two of temperature, pressure, or density must be specified for conditions after the reflected shock. See also <a href="#">T3</a> and <a href="#">P3A</a> .		
	<b>Reactor Models</b>	• Normal Reflected Shock		
RL-GAS  Reactor Property	This optional keyword is used to turn the real gas model on or off. Setting the option value to 1 will activate the real gas model if the gas reaction mechanism contains the real gas data. A value of 0 = turn OFF the real gas model and 1= turn ON the model.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Enabled</i>	Required	g/cm <sup>3</sup>	RLGAS <b>1</b>
	<b>Keyword Usage</b>	Optional keyword. By default, the real gas model is turned OFF.		
	<b>Reactor Models</b>	<ul style="list-style-type: none"><li>• Closed Homogeneous Batch Reactor</li><li>• Closed Partially Stirred Reactor</li><li>• Cylindrical Shear Flow Reactor</li><li>• Diffusion or Premixed Opposed-flow Flame</li><li>• Flame-Extinction Simulator</li><li>• Honeycomb Reactor</li><li>• IC HCCI Engine</li><li>• Multi-Zone HCCI Engine Simulator</li><li>• Normal Incident Shock</li><li>• Normal Reflected Shock</li><li>• Partially Stirred Reactor (PaSR)</li><li>• Perfectly Stirred Reactor (PSR)</li><li>• Planar Shear Flow Reactor</li><li>• Plug Flow Reactor</li><li>• Rotating Disk CVD Reactor</li><li>• SI Engine Zonal Simulator</li></ul>		

Keyword	Definition			
		• Stagnation Flow CVD Reactor		
RL-MIX  Reactor Property	This optional keyword will activate the selected real gas mixing rule if the real gas model is turned on (by RLGAS). A value of 0 = use the Van der Waals mixing rule and 1 = use the pseudocritical method (see <a href="#">Real Gas Data (p. 37)</a> ).			
	Parameters	Optional/Reqd.	Units	Examples
	Method	Required	None	RLMIX 0
	Keyword Usage	Optional keyword. By default, the van der Waals method will be applied.		
	Reactor Models	<ul style="list-style-type: none"><li>• Closed Homogeneous Batch Reactor</li><li>• Closed Partially Stirred Reactor</li><li>• Cylindrical Shear Flow Reactor</li><li>• Diffusion or Premixed Opposed-flow Flame</li><li>• Flame-Extinction Simulator</li><li>• Honeycomb Reactor</li><li>• IC HCCI Engine</li><li>• Multi-Zone HCCI Engine Simulator</li><li>• Normal Incident Shock</li><li>• Normal Reflected Shock</li><li>• Partially Stirred Reactor (PaSR)</li><li>• Perfectly Stirred Reactor (PSR)</li><li>• Planar Shear Flow Reactor</li><li>• Plug Flow Reactor</li><li>• Rotating Disk CVD Reactor</li><li>• SI Engine Zonal Simulator</li><li>• Stagnation Flow CVD Reactor</li></ul>		
ROP  Output	Inclusion of this keyword causes the rate-of-production coefficients to be printed for specified species. The keyword must be followed by one or more names of species. If any <a href="#">ROP</a> keywords are used, all the rate-of-production coefficients will be computed and written to the XML Solution File (e.g., XMLdata.zip). However, only those specified by the <a href="#">ROP</a> keyword will be printed in the diagnostic output file. More than one species may be entered per line. If the line is blank after the <a href="#">ROP</a> keyword, then all rate-of-production contributions are computed and written to the XML Solution File, but none are printed.			

Keyword	Definition			
	Keyword Usage	Optional keyword. By default, no rate-of-production values are computed.		
	Reactor Models	<ul style="list-style-type: none"><li>• Closed Homogeneous Batch Reactor</li><li>• Closed Plasma Reactor</li><li>• Honeycomb Reactor</li><li>• IC HCCI Engine</li><li>• Perfectly Stirred Reactor (PSR)</li><li>• Plasma Plug Flow Reactor</li><li>• Plasma PSR</li><li>• Plug Flow Reactor</li><li>• SI Engine Zonal Simulator</li></ul>		
	Notes	<ul style="list-style-type: none"><li>• This keyword can be added but not removed from a continuation run.</li><li>• Rates of production can be calculated for other Reactor Models through the graphical ANSYS Chemkin-Pro Post-processor</li></ul>		
RPM	Revolutions per minute of the engine crank arm.			
Reactor Property	Parameters	Optional/Reqd.	Units	Examples
	Revolutions per minute	Required	rpm	RPM <b>1200</b>
	Keyword Usage	Optional keyword. By default, the rpm is 1500.		
	Reactor Models	<ul style="list-style-type: none"><li>• IC HCCI Engine</li><li>• SI Engine Zonal Simulator</li></ul>		
RRAD	Ratio of the upper radiating disk radius to the separation distance between it and the lower substrate. This is used in calculating a surface radiation balance. <b>RRAD</b> is used only if the disk temperature is being calculated by including keyword <b>RADB</b> . See <a href="#">Equation 14.18</a> of the <a href="#">Chemkin-Pro Theory Manual</a> .			
Reactor Property	Parameters	Optional/Reqd.	Units	Examples
	Ratio of the upper radiating disk	Required	--	RRAD <b>3.0</b>
	Keyword Usage	Required keyword only if <b>RADB</b> and <b>RDSK</b> are included.		
	Reactor Models	<ul style="list-style-type: none"><li>• Rotating Disk CVD Reactor</li><li>• Stagnation Flow CVD Reactor</li></ul>		
RSHK	Inclusion of this keyword designates a reflected shock problem.			

Keyword	Definition			
Problem Type	Keyword Usage	Required keyword. See also <a href="#">ISHK</a> .		
	Reactor Models	<ul style="list-style-type: none"><li>• Normal Reflected Shock</li></ul>		
RSTR Cluster Property	Inclusion of this keyword causes ANSYS Chemkin-Pro to read a solution off the XML Solution File (e.g., XMLdata.zip) and begin iteration or integration on the current reactor conditions from this solution.			
	Keyword Usage	Optional keyword. By default, a solution is started from the user-specified conditions and no XML Solution File is used.		
	Reactor Models	<ul style="list-style-type: none"><li>• Closed Homogeneous Batch Reactor</li><li>• Closed Partially Stirred Reactor (PaSR)</li><li>• Closed Plasma Reactor</li><li>• Cylindrical Shear Flow Reactor</li><li>• Diffusion or Premixed Opposed-flow Flame</li><li>• Honeycomb Reactor</li><li>• IC HCCI Engine</li><li>• Partially Stirred Reactor (PaSR)</li><li>• Perfectly Stirred Reactor (PSR)</li><li>• Planar Shear Flow Reactor</li><li>• Plasma Plug Flow Reactor</li><li>• Plasma PSR</li><li>• Plug Flow Reactor</li><li>• Premixed Laminar Burner-stabilized Flame</li><li>• Premixed Laminar Flame-speed Calculation</li><li>• Rotating Disk CVD Reactor</li><li>• SI Engine Zonal Simulator</li><li>• Stagnation Flow CVD Reactor</li></ul>		
RTIM Solver	Relative tolerance for convergence of Newton iteration as it is used in the pseudo time stepping procedure for steady-state problems employing the <i>Twopnt</i> solver. Since we are not seeking accuracy in a transient solution, this convergence criteria typically does not need to be as stringent as for the Newton iteration on the actual steady-state solution.			
	Parameters	Optional/Reqd.	Units	Examples
	Absolute tolerance	Required	--	RTIM <b>1.E-3</b>



Keyword	Definition			
	Keyword Usage	Optional keyword. By default, the relative tolerance is 1.E-4. See also <a href="#">ATIM</a> .		
	Reactor Models	<ul style="list-style-type: none"><li>• Closed Plasma Reactor</li><li>• Cylindrical Shear Flow Reactor</li><li>• Diffusion or Premixed Opposed-flow Flame</li><li>• Honeycomb Reactor</li><li>• Non-reactive Gas Mixer</li><li>• Perfectly Stirred Reactor (PSR)</li><li>• Planar Shear Flow Reactor</li><li>• Plasma PSR</li><li>• Premixed Laminar Burner-stabilized Flame</li><li>• Premixed Laminar Flame-speed Calculation</li><li>• Rotating Disk CVD Reactor</li><li>• Stagnation Flow CVD Reactor</li></ul>		
	Notes	<ul style="list-style-type: none"><li>• For a more precise definition, see the description of <a href="#">RTOL</a>.</li></ul>		
RTIME  Reactor Property	Turn on or off solution of the residence-time equation for a plug-flow simulation.			
	Parameters	Optional/Reqd.	Units	Examples
	String “ON” or “OFF” to toggle the momentum equation	Required	--	RTIME <b>ON</b>  RTIME OFF
	Keyword Usage	Optional keyword. By default, the residence-time equation is solved (ON).		
	Reactor Models	<ul style="list-style-type: none"><li>• Honeycomb Reactor</li><li>• Plasma Plug Flow Reactor</li><li>• Plug Flow Reactor</li></ul>		
RTLTM  Solver	A different relative tolerance can be assigned to moment variables in steady-state calculations. By default, the same relative tolerance given by <a href="#">RTOL</a> is used for all variables.			
	Parameters	Optional/Reqd.	Units	Examples
	Tolerance	Required	--	RTLTM <b>1.0E-4</b>
	Keyword Usage	Optional keyword. By default, the absolute tolerance is determined by <a href="#">RTOL</a> .		

Keyword	Definition			
	<b>Reactor Models</b>	<ul style="list-style-type: none"><li>• Closed Plasma Reactor</li><li>• Cylindrical Shear Flow Reactor</li><li>• Perfectly Stirred Reactor (PSR)</li><li>• Planar Shear Flow Reactor</li><li>• Plasma PSR</li></ul>		
<b>RTLS</b>  Solver	Relative tolerance used by the transient solver, DASPK, as an indicator of the accuracy desired in the solution for the sensitivity coefficients only. Generally, the sensitivity coefficients need not be solved to a great degree of accuracy, so these tolerances should be lower than the tolerances placed on the physical variables.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Relative tolerance</i>	Required	--	RTLS <b>1.E-2</b>
	<b>Keyword Usage</b>	Optional keyword. By default, the relative tolerance is 1.E-5.		
	<b>Reactor Models</b>	<ul style="list-style-type: none"><li>• Closed Homogeneous Batch Reactor</li><li>• Closed Plasma Reactor</li><li>• Honeycomb Reactor</li><li>• IC HCCI Engine</li><li>• Perfectly Stirred Reactor (PSR)</li><li>• Plasma PSR</li><li>• Plasma Plug Flow Reactor</li><li>• Plug Flow Reactor</li><li>• SI Engine Zonal Simulator</li></ul>		
<b>RTOL</b>  Solver	Relative tolerance used by the solver to determine convergence and as an indicator of the accuracy desired in the physical solution. In general the value of <b>RTOL</b> roughly corresponds to the number of significant digits that should be expected from a solution. A typical value should be between 10-3 and 10-6, which would provide roughly three to six significant digits.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Relative tolerance</i>	Required	--	RTOL <b>1.E-3</b>
	<b>Keyword Usage</b>	Optional keyword. The default values are:  Open 0-D Reactors run in steady-state mode, Opposed-flow Flame, Premixed Laminar Burner-stabilized Flame, Premixed Laminar Flame-speed Calculation, Shear Flow Reactor: 1.E-4		

Keyword	Definition			
		Normal Incident Shock, Normal Reflected Shock, Plug Flow Reactor, Partially Stirred Reactor (PaSR), CVD: 1.E-6  Closed 0-D Reactors and Open 0-D Reactors run in transient mode: 1.E-8  See also <a href="#">ATOL</a> .		
	Reactor Models	<ul style="list-style-type: none"><li>• Closed Homogeneous Batch Reactor</li><li>• Closed Partially Stirred Reactor (PaSR)</li><li>• Closed Plasma Reactor</li><li>• Cylindrical Shear Flow Reactor</li><li>• Diffusion or Premixed Opposed-flow Flame</li><li>• Honeycomb Reactor</li><li>• IC HCCI Engine</li><li>• Non-reactive Gas Mixer</li><li>• Normal Incident Shock</li><li>• Normal Reflected Shock</li><li>• Opposed-flow Flame</li><li>• Partially Stirred Reactor (PaSR)</li><li>• Perfectly Stirred Reactor (PSR)</li><li>• Planar Shear Flow Reactor</li><li>• Plasma PSR</li><li>• Plug Flow Reactor</li><li>• Premixed Laminar Burner-stabilized Flame</li><li>• Premixed Laminar Flame-speed Calculation</li><li>• Rotating Disk CVD Reactor</li><li>• SI Engine Zonal Simulator</li><li>• Stagnation Flow CVD Reactor</li></ul>		
SCAT  Output	Request the scatter plot of a scalar to be output to the file <i>scatter.plt</i> .			
	Parameters	Optional/Reqd.	Units	Examples
	Scalar (temperature or species name)	Required	--	SCAT <b>CH4</b>

Keyword	Definition			
	Keyword Usage	Optional keyword. By default, no scatter plot is printed.		
	Reactor Models	<ul style="list-style-type: none"><li>Closed Partially Stirred Reactor (PaSR)</li><li>Partially Stirred Reactor (PaSR)</li></ul>		
SCCM	The volumetric flow rate into the reactor for an optionally specified inlet stream, in standard cubic centimeters per minute assuming that the inlet temperature is 298.15 K and the inlet pressure is 1 atm unless a different value for TSCCM is provided.			
Inlet Property	Parameters	Optional/Reqd.	Units	Examples
	Inlet stream name	Optional  If there is no stream name than the volumetric flow rate applies to the default or all defined streams.	--	SCCM <b>secondary_air</b> 300
	Equivalent volumetric flow rate at standard conditions	Required	standard cm <sup>3</sup> /min	SCCM secondary_air <b>300</b>
	Keyword Usage	PSRs and PaSRs: Optional keyword. If none of TAU, FLRT / FPRO, SCCM / SCCMPRO are specified or are nonzero, then a closed-system is assumed. FLRT / FPRO or SCCM / SCCMPRO is required for each INLET stream defined.  Stagnation Flow CVD Reactors: FLRT / FPRO or SCCM / SCCMPRO or UINL is required for each inlet stream defined.  Rotating Disk CVD Reactors: Optional keyword.		
	Reactor Models	<ul style="list-style-type: none"><li>Non-reactive Gas Mixer</li><li>Perfectly Stirred Reactor (PSR)</li><li>Plasma PSR</li><li>Rotating Disk CVD Reactor</li><li>Stagnation Flow CVD Reactor</li></ul>		

Keyword	Definition			
Inlet Property Profiles	<b>SCCMPRO</b> Used to specify a transient profile or function of mass flow rate vs. time for an inlet stream, in standard cubic centimeters per minute assuming that the inlet temperature is 298.15 K and the inlet pressure is 1 atm unless a different standard temperature ( <b>TSCCM</b> ) is entered. The profile specified will be interpolated linearly from the <b>SCCMPRO</b> points provided.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Inlet stream name</i>	Optional  If no stream name is given, the profile described by the reactant and mole fraction is assumed to apply to all reactors in a cluster.	--	SCCMPRO <b>purge</b> 0.19 300
	<i>Time</i>	Required	sec (cm for flow reactors)	SCCMPRO <b>0.19</b> 300
	<i>Equivalent volumetric flow rate at standard conditions</i>	Required	standard cm <sup>3</sup> /min	SCCMPRO 0.19 <b>300</b>
<b>Keyword Usage</b>		<p><b>PFRs and Monolith Reactors:</b> Flow specification via one of <b>VEL</b>, <b>VDOT</b>, <b>VDOTPRO</b> <b>SCCM</b> <b>SCCMPRO</b> <b>FLRT</b>, or <b>FPRO</b> is required.</p> <p>PSRs and PaSRs: Optional keyword. If none of <b>TAU</b>, <b>FLRT</b> / <b>FPRO</b>, <b>SCCM</b> / <b>SCCMPRO</b> are specified or are nonzero, then a closed-system is assumed. <b>FLRT</b> / <b>FPRO</b> or <b>SCCM</b> / <b>SCCMPRO</b> is required for each <b>INLET</b> stream defined.</p> <p>Stagnation Flow CVD Reactors: <b>FLRT</b> / <b>FPRO</b> or <b>SCCM</b> / <b>SCCMPRO</b> or <b>UINL</b> is required for each inlet stream defined.</p> <p>Rotating Disk CVD Reactors: Optional keyword.</p>		

Keyword	Definition			
	<b>Reactor Models</b>	<ul style="list-style-type: none"><li>• Honeycomb Monolith Reactor</li><li>• Non-reactive Gas Mixer</li><li>• Perfectly Stirred Reactor (PSR)</li><li>• Plasma PFR</li><li>• Plasma PSR</li><li>• Plug Flow Reactor</li><li>• Rotating Disk CVD Reactor</li><li>• Stagnation Flow CVD Reactor</li></ul>		
<b>SCLM</b>  Reactor Property	Scaling factor for the particles moments (moments method) or number density (sectional method). A non-unity value for this parameter changes the units of the (internal) solution variable for particle moments or number density. For example, setting it to 1.0E+06 results in micro-moles whereas setting it to 1.0E+09 means that it is nano-moles. A value of 1 would mean that the unit should be moles. A recommended value for typical problems is 1.0E+12. Such scaling helps preserve the positivity of the solution during numerical computation.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Scaling factor</i>	Required	--	SCLM 1.0E+12
	<b>Keyword Usage</b>	Optional keyword.		
	<b>Reactor Models</b>	<ul style="list-style-type: none"><li>• Closed Homogeneous Batch Reactor</li><li>• Closed Plasma Reactor</li><li>• Flame-Extinction Simulator</li><li>• Honeycomb Monolith Reactor</li><li>• IC HCCI Engine</li><li>• Multi-Zone HCCI Engine Simulator</li><li>• Opposed-flow Flame</li><li>• Perfectly Stirred Reactor (PSR)</li><li>• Plasma Plug Flow Reactor</li><li>• Plasma PSR</li><li>• Plug Flow Reactor</li><li>• Premixed Laminar Burner-stabilized Flame</li><li>• Premixed Laminar Flame-speed Calculation</li><li>• SI Engine Zonal Simulator</li></ul>		

Keyword	Definition			
		• Stagnation Flow Flame Simulator		
SCLS  Reactor Property	Scaling factor for the particle surface species concentrations. A non-unity value for this parameter changes the units of the (internal) solution variable for particle surface species. For example, setting it to 1.0E+06 results in micro-moles whereas setting it to 1.0E+09 means that it is nano-moles. A value of 1 would mean that the unit should be moles. A recommended value for typical problems is 1.0E+12. Such scaling helps preserve the positivity of the solution during numerical computation.			
	Parameters	Optional/Reqd.	Units	Examples
	Scaling factor	Required	--	SCLS 1.0E+12
	Keyword Usage	Optional keyword.		
	Reactor Models	<ul style="list-style-type: none"><li>• Closed Homogeneous Batch Reactor</li><li>• Closed Plasma Reactor</li><li>• Flame-Extinction Simulator</li><li>• Honeycomb Monolith Reactor</li><li>• IC HCCI Engine</li><li>• Multi-Zone HCCI Engine Simulator</li><li>• Opposed-flow Flame</li><li>• Perfectly Stirred Reactor (PSR)</li><li>• Plasma Plug Flow Reactor</li><li>• Plasma PSR</li><li>• Plug Flow Reactor</li><li>• Premixed Laminar Burner-stabilized Flame</li><li>• Premixed Laminar Flame-speed Calculation</li><li>• SI Engine Zonal Simulator</li><li>• Stagnation Flow Flame Simulator</li></ul>		
SCOR  Solver	Flag instructing that the transient solver, DASPK will use staggered corrector method to solve sensitivity equations. The staggered corrector method is the sensitivity method that was used in previous versions of ANSYS Chemkin-Pro and is mainly provided for backwards compatibility. It is generally slower than the default sensitivity method in Chemkin-Pro (which is the staggered direct method) but sometimes can be more stable and robust than the staggered direct method.			
	Keyword Usage	Optional keyword. By default, DASPK uses staggered corrector method to solve sensitivity equations.		
	Reactor Models	<ul style="list-style-type: none"><li>• Closed Homogeneous Batch Reactor</li></ul>		

Keyword	Definition			
		<ul style="list-style-type: none"><li>• Closed Plasma Reactor</li><li>• Honeycomb Reactor</li><li>• IC HCCI Engine</li><li>• Non-reactive Gas Mixer</li><li>• Perfectly Stirred Reactor (PSR)</li><li>• Plasma PSR</li><li>• Plasma Plug Flow Reactor</li><li>• Plug Flow Reactor</li><li>• SI Engine Zonal Simulator</li></ul>		
	Notes	<ul style="list-style-type: none"><li>• SCOR can be changed for a continuation run, but it cannot be removed from one.</li></ul>		
SCOV  Output	Analyze the coverage dependence of a surface reaction, i.e., create a table of effective reaction rates versus temperature. Surface coverage is assumed to be that of the bath-gas composition. The ALL option is the default and produces tables for every surface reaction. The NONE option suppresses output for all of the reactions. If reaction information is desired for only certain reactions, they may be optionally specified by their number (given in the Pre-processor output) or by typing an exact duplicate of the reaction expression (see example input).			
	Parameters	Optional/Reqd.	Units	Examples
	ALL option	Optional, default is ALL	--	SCOV ALL
	NONE option	Optional, default is ALL	--	SCOV NONE
	Surface reaction number list	Optional, default is ALL	--	SCOV 2 5
	Surface reaction expression	Optional, default is ALL	--	SCOV CH(S)+H<=>C(S,R)+H2
	Keyword Usage	Optional keyword. By default, the table output is determined by the ALL or NONE keyword.		
Reactor Models	<ul style="list-style-type: none"><li>• Mechanism Analyzer</li></ul>			



Keyword	Definition	
<b>SENG</b> Output	Inclusion of this keyword causes the calculation of the first-order sensitivity coefficients, with respect to the gas-phase and surface chemistry rate constants, for the growth rate of all bulk phases. Growth-rate sensitivities will be included in the printed output and the XML Solution File (e.g., XMLdata.zip).	
	<b>Keyword Usage</b>	Optional keyword. By default, no sensitivity coefficients are computed. See also <a href="#">ASEN</a> .
	<b>Reactor Models</b>	<ul style="list-style-type: none"> <li>• Closed Homogeneous Batch Reactor</li> <li>• Closed Plasma Reactor</li> <li>• Honeycomb Reactor</li> <li>• Perfectly Stirred Reactor (PSR)</li> <li>• Plasma Plug Flow Reactor</li> <li>• Plasma PSR</li> <li>• Plug Flow Reactor</li> </ul>
	<b>Notes</b>	<ul style="list-style-type: none"> <li>• This keyword can be added but not removed from a continuation run.</li> </ul>
<b>SENT</b> Output	Calculate and store sensitivity coefficients for gas temperature with respect to reaction A-factors. See <a href="#">ASEN</a> .	
	<b>Keyword Usage</b>	Optional keyword. By default, no sensitivity coefficients are computed or printed. Same as <a href="#">ASEN TEMP</a> .
	<b>Reactor Models</b>	<ul style="list-style-type: none"> <li>• Closed Homogeneous Batch Reactor</li> <li>• Closed Plasma Reactor</li> <li>• Honeycomb Reactor</li> <li>• IC HCCI Engine</li> <li>• Multi-Zone HCCI Engine Simulator</li> <li>• Perfectly Stirred Reactor (PSR)</li> <li>• Plasma Plug Flow Reactor</li> <li>• Plasma PSR</li> <li>• Plug Flow Reactor</li> <li>• Opposed-flow Flame</li> <li>• Premixed Laminar Burner-stabilized Flame</li> <li>• Premixed Laminar Flame-speed Calculation</li> <li>• Rotating Disk CVD Reactor</li> </ul>

Keyword	Definition			
		<ul style="list-style-type: none"><li>• SI Engine Zonal Simulator</li><li>• Stagnation Flow CVD Reactor</li></ul>		
SFAC  Reactor Property	This keyword specifies that the rates of all surface reactions will be multiplied (scaled) by the factor SFAC. This option is sometimes useful if convergence difficulties are encountered due to unusually large reaction rates. The problem would be first solved with artificially reduced reaction rates, which then can be increased in subsequent continuations or restarts until SFAC is one.			
	Parameters	Optional/Reqd.	Units	Examples
	Multiplier value	Required	--	SFAC <b>2.0</b>
	Reactor number (PSR clusters only)	Optional  If no number is given, value is assumed to apply to all reactors in a cluster.	--	SFAC 2.0 <b>1</b>
	Keyword Usage	Optional keyword. By default, the multiplier value is set to 1.0.		
	Reactor Models	<ul style="list-style-type: none"><li>• Closed Homogeneous Batch Reactor</li><li>• Closed Plasma Reactor</li><li>• Cylindrical Shear Flow Reactor</li><li>• Honeycomb Reactor</li><li>• Non-reactive Gas Mixer</li><li>• Perfectly Stirred Reactor (PSR)</li><li>• Planar Shear Flow Reactor</li><li>• Plasma Plug Flow Reactor</li><li>• Plasma PSR</li><li>• Plug Flow Reactor</li><li>• Rotating Disk CVD Reactor</li><li>• Stagnation Flow CVD Reactor</li></ul>		
SFLR	Sometimes during the solution procedure some of the very small gas-phase mass fractions, surface site fractions, or bulk species fractions may be calculated as a			

Keyword	Definition			
Solver	slightly negative number. No solution component will be allowed to drop below the floor value specified by <b>SFLR</b> .			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Minimum bounds on the solution variables</i>	Required	--	<b>SFLR -1.E-5</b>
	<b>Keyword Usage</b>	Optional keyword. By default, the minimum bounds on the solution variables is set to -1.E-4		
	<b>Reactor Models</b>	<ul style="list-style-type: none"><li>• Diffusion or Premixed Opposed-flow Flame</li><li>• Non-reactive Gas Mixer</li><li>• Perfectly Stirred Reactor (PSR)</li><li>• Plasma PSR</li><li>• Rotating Disk CVD Reactor</li><li>• Stagnation Flow CVD Reactor</li><li>• Premixed Laminar Burner-stabilized Flame</li><li>• Premixed Laminar Flame-speed Calculation</li></ul>		
<b>SFMN</b> Solver	Set the minimum bounds of the surface species concentration to a slightly negative number to allow the solver more room to search for a solution.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Minimum bound</i>	Required	--	<b>SFMN -1.0d-06</b>
	<b>Keyword Usage</b>	Optional keyword. Usable only with Particle Tracking.		
	<b>Reactor Models</b>	<ul style="list-style-type: none"><li>• Opposed-flow Flame</li><li>• Premixed Laminar Burner-stabilized Flame</li><li>• Premixed Laminar Flame-speed Calculation</li></ul>		
<b>SGMAXIT</b> Solver	This controls the maximum number of iterations the segregated solver can take per step to solve the problem. The default is 100 and you may increase this value to give the solver greater chance to solve your problem if it is very hard to solve.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Scaling factor</i>	Required	--	<b>SGMAXIT 100</b>
	<b>Keyword Usage</b>	Optional keyword.		
	<b>Reactor Models</b>	<ul style="list-style-type: none"><li>• Diffusion or Premixed Opposed-flow Flame</li><li>• Opposed-flow Flame</li><li>• Premixed Laminar Burner-stabilized Flame</li><li>• Premixed Laminar Flame-speed Calculation</li></ul>		

Keyword	Definition			
SG-TOL  Solver	Absolute tolerance criterion on gas-phase mole fractions in segregated scheme.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Absolute tolerance</i>	Required	--	SGTOL 1.0E-10
	<b>Keyword Usage</b>	Optional keyword. The default value is 1E-10.		
	<b>Reactor Models</b>	<ul style="list-style-type: none"><li>• Diffusion or Premixed Opposed-flow Flame</li><li>• Opposed-flow Flame</li><li>• Premixed Laminar Burner-stabilized Flame</li><li>• Premixed Laminar Flame-speed Calculation</li></ul>		
SIDR  Solver	Turns on the multi-zone SI Engine Zonal simulation with gas-phase chemistry de-activated. The number of zones is set to 2 by default. <b>SIKN</b> and <b>SIDR</b> are mutually exclusive.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Number of zones</i>	Required	--	SIDR 2
	<b>Keyword Usage</b>	Optional keyword.		
	<b>Reactor Models</b>	<ul style="list-style-type: none"><li>• SI Engine Zonal Simulator</li></ul>		
SIKN  Solver	Turns on the multi-zone SI Engine Zonal simulation with gas-phase chemistry activated. The number of zones is set to 2 by default. <b>SIKN</b> and <b>SIDR</b> are mutually exclusive.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Number of zones</i>	Required	--	SIKN 2
	<b>Keyword Usage</b>	Optional keyword.		
	<b>Reactor Models</b>	<ul style="list-style-type: none"><li>• SI Engine Zonal Simulator</li></ul>		
SIOA  Reactor Property	Specifies the crank angle when the SI Engine Zonal Simulator properties will be saved to the XML solution file.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>crank_angle</i>	Required	degree	SIOA <b>5.1</b>
	<b>Keyword Usage</b>	Optional keyword.		
	<b>Reactor Models</b>	<ul style="list-style-type: none"><li>• SI Engine Zonal Simulator</li></ul>		
SIZE  Output	Use this keyword to set the data block size in bytes for the XML Solution File (e.g., <i>XMLdata.zip</i> ). Changing this value may affect the performance of the XML parsing routines in the graphical ANSYS Chemkin-Pro Post-processor.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Data block size</i>	Required	bytes	SIZE <b>10000000</b>
	<b>Keyword Usage</b>	Optional keyword. By default, the data block size is 10 MB.		
	<b>Reactor Models</b>	<ul style="list-style-type: none"><li>• Chemical and Phase Equilibrium Calculations</li></ul>		

Keyword	Definition		
	<ul style="list-style-type: none"><li>• Closed Homogeneous Batch Reactor</li><li>• Closed Partially Stirred Reactor (PaSR)</li><li>• Closed Plasma Reactor</li><li>• Cylindrical Shear Flow Reactor</li><li>• Diffusion or Premixed Opposed-flow Flame</li><li>• Honeycomb Reactor</li><li>• IC HCCI Engine</li><li>• Mechanism Analyzer</li><li>• Non-reactive Gas Mixer</li><li>• Normal Incident Shock</li><li>• Normal Reflected Shock</li><li>• Partially Stirred Reactor (PaSR)</li><li>• Perfectly Stirred Reactor (PSR)</li><li>• Planar Shear Flow Reactor</li><li>• Plasma Plug Flow Reactor</li><li>• Plasma PSR</li><li>• Plug Flow Reactor</li><li>• Premixed Laminar Burner-stabilized Flame</li><li>• Premixed Laminar Flame-speed Calculation</li><li>• Rotating Disk CVD Reactor</li><li>• SI Engine Zonal Simulator</li><li>• Stagnation Flow CVD Reactor</li></ul>		
<b>SLIP</b>	Use the slip velocity model to calculate axial velocity at wall when Knudsen number is large. The model calculates the axial velocity at wall as		
Reactor Property	$U_{wall}=C \cdot L \cdot \left(\frac{2-\Sigma_v}{\Sigma_v}\right) \cdot \frac{dU}{dy}$ where $L$ is the characteristic length, $U$ is the axial velocity, $C$ is the multiplier, $\Sigma_v$ is the tangential momentum accommodation coefficient.		
	Parameters	Optional/Reqd.	Units
	Multiplier	Required	--
	Tangential momentum	Required	--
	Examples		
	SLIP <b>3.0</b> 0.9		
	SLIP 3.0 <b>0.9</b>		

Keyword	Definition			
	<i>accommodation coefficient</i>			
	<b>Keyword Usage</b>	Optional keyword. By default, the slip velocity model is not used.		
	<b>Reactor Models</b>	<ul style="list-style-type: none"><li>• Cylindrical Shear Flow Reactor</li><li>• Planar Shear Flow Reactor</li></ul>		
<b>SOLUTION</b>  _TECHNIQUE Solver	Controls the underlying solution technique. Previous versions of ANSYS Chemkin-Pro use an older and generally less robust solution method. By default, solution_technique is set to 1, which means the new and generally more robust (and for larger mechanisms often faster) technique is used. Setting solution_technique to 0 uses the older method and you should only use this if you are having convergence issues with <i>CHEMKIN-Pro</i> and are confident you do not have any problems with your mechanism or problem specification.			
	<b>Keyword Usage</b>	Optional keyword. By default, SOLUTION_TECHNIQUE is set to 1.		
	<b>Reactor Models</b>	<ul style="list-style-type: none"><li>• Closed Homogeneous Batch Reactor</li><li>• Closed Plasma Reactor</li><li>• Honeycomb Reactor</li><li>• IC HCCI Engine</li><li>• Multi-Zone HCCI Engine Simulator</li><li>• Perfectly Stirred Reactor (PSR)</li><li>• Plasma Plug Flow Reactor</li><li>• Plasma PSR</li><li>• Plug Flow Reactor</li><li>• Opposed-flow Flame</li><li>• Premixed Laminar Burner-stabilized Flame</li><li>• Premixed Laminar Flame-speed Calculation</li><li>• SI Engine Zonal Simulator</li></ul>		
<b>SP</b>	Constant pressure and entropy constraints.			
Problem Type	<b>Keyword Usage</b>	Optional keyword. Exactly one problem-type keyword must be included.		
	<b>Reactor Models</b>	<ul style="list-style-type: none"><li>• Chemical and Phase Equilibrium Calculations</li></ul>		
	<b>Notes</b>	<ul style="list-style-type: none"><li>• <b>PS</b> keyword.is equivalent.</li></ul>		

Keyword	Definition			
SPOS  Solver	This keyword provides a (small positive) number that will replace any negative species mass or site fractions. The replacement is made after every successful sequence of time steps, upon adding mesh points, and on restart or continuation. SPOS is often helpful in starting difficult problems when the initial guess is far from the solution. SPOS attempts to force the transient solution away from nonphysical regions that may otherwise be entered due to bad initial conditions and badly conditioned systems.			
	Parameters	Optional/Reqd.	Units	Examples
	Species mass fraction	Required	--	SPOS <b>1.E-14</b>
	Keyword Usage	Optional keyword. By default, no substitution is made for negative fractions during solution for all Reactor Models except for Opposed-flow Flames, where the default value is 1.E-10.		
	Reactor Models	<ul style="list-style-type: none"><li>• Diffusion or Premixed Opposed-flow Flame</li><li>• Non-reactive Gas Mixer</li><li>• Perfectly Stirred Reactor (PSR)</li><li>• Plasma PSR</li><li>• Premixed Laminar Burner-stabilized Flame</li><li>• Premixed Laminar Flame-speed Calculation</li><li>• Rotating Disk CVD Reactor</li><li>• Stagnation Flow CVD Reactor</li></ul>		
SQRX  Solver	A pseudo wall thermal conductivity to allow surface enthalpy production to "overflow" in the downstream direction. This keyword is useful when the reactor model fails to converge repeatedly because of stiff surface chemistry and the reactor wall temperature is not fixed. The overall enthalpy of the reactor is still conserved because this pseudo wall enthalpy flux is included in the energy equation.			
	Parameters	Optional/Reqd.	Units	Examples
	Pseudo conductivity	Required	--	SQRX <b>0.001</b>
	Keyword Usage	Optional keyword. By default, no thermal conduction in wall is considered.		
	Reactor Models	<ul style="list-style-type: none"><li>• Cylindrical Shear Flow Reactor</li><li>• Planar Shear Flow Reactor</li></ul>		
SRXN  Output	Prints out a table of reaction rates and other pertinent information for a surface reaction. The ALL option is the default and produces tables for every surface reaction. The NONE option suppresses output for all of the reactions. If reaction information is desired for only certain reactions, they may be optionally specified			

Keyword	Definition			
	by their number (given in the Pre-processor output) or by typing an exact duplicate of the reaction expression (see example input).			
	Parameters	Optional/Reqd.	Units	Examples
	<i>ALL option</i>	<b>Optional, default is ALL</b>	--	SRXN <b>ALL</b>
	<i>NONE option</i>	<b>Optional, default is ALL</b>	--	SRXN <b>NONE</b>
	<i>Surface reaction number list</i>	<b>Optional, default is ALL</b>	--	SRXN <b>2 5</b>
	<i>Surface reaction expression</i>	<b>Optional, default is ALL</b>	--	SRXN <b>CH(S)+H&lt;=&gt;C(S,R)+H2</b>
	<b>Keyword Usage</b>	Optional keyword. By default, the table output is determined by the <a href="#">ALL</a> or <a href="#">NONE</a> keyword.		
	<b>Reactor Models</b>	• Mechanism Analyzer		
<b>SS-DR</b>	The nominal value of the Stoichiometric Scalar Dissipation Rate (SSDR). The first flamelet will be computed for this value.			
Reactor Property	Parameters	Optional/Reqd.	Units	Examples
	<i>Nominal value of SSDR</i>	Required	1/s	SSDR <b>1.0</b>
	<b>Keyword Usage</b>	Optional keyword.		
	<b>Reactor Models</b>	• Diffusion Flamelet Generator		
<b>SS-DR_MAX</b>	The maximum value of the Stoichiometric Scalar Dissipation Rate (SSDR). After computing a flamelet for the nominal value (specified by keyword SSDR), continuations to SSDR_MAX are done in a number of steps as specified by keyword NSTEP_HIGH.			
Reactor Property	Parameters	Optional/Reqd.	Units	Examples
	<i>Maximum value of SSDR</i>	Optional	1/s	SSDR_MAX <b>100</b>
	<b>Keyword Usage</b>	Optional keyword.		
	<b>Reactor Models</b>	• Diffusion Flamelet Generator		
<b>SS-DR_MIN</b>	The minimum value of the Stoichiometric Scalar Dissipation Rate (SSDR). After computing a flamelet for the nominal value (specified by keyword SSDR), continuations to SSDR_MIN are done in a number of steps as specified by keyword NSTEP_LOW.			
Reactor Property				



Keyword	Definition			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Minimum value of SSDR</i>	Optional	1/s	SSDR_MIN <b>0.001</b>
	<b>Keyword Usage</b>	Optional keyword.		
	<b>Reactor Models</b>	• Diffusion Flamelet Generator		
<b>SSKIP</b>	Skip the initial surface site fraction calculation.			
Solver	<b>Keyword Usage</b>	Optional keyword. By default, an initial solution is performed to determine the surface site fractions holding the reagent gas species constant.		
	<b>Reactor Models</b>	• Honeycomb Monolith Reactor  • Plasma Plug Flow Reactor  • Plug Flow Reactor		
<b>SS-MAX-ITER</b>	The maximum number of iterations per steady state search, in the steady-state solver TWOPNT. This is the maximum number of iterations that are allowed each time TWOPNT searches to find the steady state solution. Typically you will not need to change this maximum because TWOPNT will revert to its time stepping algorithm and then re-try searching for the steady state.			
Solver	Parameters	Optional/Reqd.	Units	Examples
	<i>Maximum steady state iterations</i>	Optional	--	SSMAXITER <b>120</b>
	<b>Keyword Usage</b>	Optional keyword. By default, the maximum number of iterations is 100.		
	<b>Reactor Models</b>	• Cylindrical Shear Flow Reactor  • Diffusion or Premixed Opposed-flow Flame  • Non-reactive Gas Mixer  • Perfectly Stirred Reactor (PSR)  • Planar Shear Flow Reactor  • Plasma PSR  • Premixed Laminar Burner-stabilized Flame  • Premixed Laminar Flame-speed Calculation  • Rotating Disk CVD Reactor  • Stagnation Flow CVD Reactor		
	<b>Notes</b>	• SSMAXITER must be >=1.		

Keyword	Definition			
SS-RX  Solver	A pseudo diffusivity for surface species to allow them to diffuse along the wall surface in the downstream direction. This keyword is useful when the reactor model fails to converge repeatedly because of stiff surface chemistry and the reactor wall temperature is fixed. The overall mass and element conservations of the reactor are still satisfied because pseudo surface species fluxes are included in the surface species equations.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Pseudo conductivity</i>	Required	--	SSRX <b>0.0001</b>
	Keyword Usage	Optional keyword. By default, no surface species flux on wall is considered.		
	Reactor Models	<ul style="list-style-type: none"><li>Cylindrical Shear Flow Reactor</li><li>Planar Shear Flow Reactor</li></ul>		
	Notes	<ul style="list-style-type: none"><li>Typically, the value of SSRX should be kept under 0.01.</li></ul>		
SSTT  Solver	Inclusion of this keyword indicates that the local sensitivity analysis will be performed instead of the integrated sensitivity analysis for transient or plug-flow calculations. This may be helpful in speeding up calculations of sensitivity, but we caution that the local sensitivity is less accurate than the integrated sensitivity.			
	Keyword Usage	Optional keyword. By default, the integrated sensitivity analysis will be performed for transient calculations when sensitivity data is requested.		
	Reactor Models	<ul style="list-style-type: none"><li>Closed Homogeneous Batch Reactor</li><li>Closed Plasma Reactor</li><li>Honeycomb Reactor</li><li>IC HCCI Engine</li><li>Perfectly Stirred Reactor (PSR)</li><li>Plasma PSR</li><li>Plasma Plug Flow Reactor</li><li>Plug Flow Reactor</li><li>SI Engine Zonal Simulator</li></ul>		
	Notes	<ul style="list-style-type: none"><li><a href="#">SSTT</a> can be added to a continuation run, but it cannot be removed from one.</li></ul>		
	STAG  Problem Type	Specify a Stagnation Flow CVD Reactor model.		
		Keyword Usage	Required keyword. See also <a href="#">OMEG</a> . If the keyword <a href="#">STAG</a> is given and the spin rate <a href="#">OMEG</a> is nonzero, then this inconsistent input will generate an error. A	

Keyword	Definition			
		stagnation-point flow can also be specified by using "OMEG 0".		
	Reactor Models	• Stagnation Flow CVD Reactor		
STAG- NA- TION  _FLAME Problem Type	Indicates Burner-stabilized Stagnation Flow problem type.			
	Keyword Usage	Required keyword.		
	Reactor Models	• Premixed Laminar Burner-stabilized Stagnation Flow Flame Simulator		
STCH  Reactor Property	Parameter to produce a non-uniform grid. For cartesian coordinates the initial grid location for a node J is $X(J)=A*(J-1)**STCH$ , where $A=HITE/(NPTS-1)**STCH$ , HITE is the reactor height, and NPTS is the total number of grid nodes. If STCH=1, a uniform grid is produced. For STCH > 1, the grid is more tightly spaced at the lower boundary (cartesian-coordinates) or at the outer boundary ( cylindrical coordinates), and consequently the grid is more widely spaced at the other boundary.			
	Parameters	Optional/Reqd.	Units	Examples
	Cartesian coordinates	Required	--	STCH 1.2
	Keyword Usage	Optional keyword. By default, the program is set to 1.		
	Reactor Models	• Cylindrical Shear Flow Reactor  • Planar Shear Flow Reactor		
STCK  Output	Analyzes the forward and reverse surface reaction's sticking coefficient, if applicable. The ALL option is the default and produces tables for every surface reaction with a sticking-coefficient formulation. The NONE option suppresses output for all of the reactions. If reaction information is desired for only certain reactions, they may be optionally specified by their number (given in the Pre-processor output) or by typing an exact duplicate of the reaction expression (see example input).			
	Parameters	Optional/Reqd.	Units	Examples
	ALL option	Optional, default is ALL	--	STCK ALL
	NONE option	Optional, default is ALL	--	STCK NONE
	Surface reaction number list	Optional, default is ALL	--	STCK 2 5

Keyword	Definition			
	Surface reaction expression	Optional, default is ALL	--	STCK <b>CH(S)+H&lt;=&gt;C(S,R)+H2</b>
	Keyword Usage	Optional keyword. By default, the table output is determined by the <a href="#">ALL</a> or <a href="#">NONE</a> keyword.		
	Reactor Models	• Mechanism Analyzer		
STPO Solver	Initial time step size used by the steady-state solver <i>Twopnt</i> during the initial calculation for the surface conditions at the inlet.			
	Parameters	Optional/Reqd.	Units	Examples
	Initial time step	Required	cm	STPO <b>1.0E-7</b>
	Keyword Usage	Optional keyword. By default, the initial time step is 1.0E-6.		
	Reactor Models	• Cylindrical Shear Flow Reactor  • Planar Shear Flow Reactor		
STPT Solver	The maximum internal time step for the solver in transient calculations. <a href="#">STPT</a> determines the largest time-step the transient solver can take at one time and thereby controls the resolution for interpolation of specified time-profiles.			
	Parameters	Optional/Reqd.	Units	Examples
	Time step	Required	sec	STPT <b>1.0E-4</b>
	Aurora Usage	Optional keyword. If not specified, then If either <a href="#">DELT</a> or <a href="#">DTSV</a> are specified, <a href="#">STPT</a> is set to the smallest of these values. If neither <a href="#">DELT</a> nor <a href="#">DTSV</a> are specified, then <a href="#">STPT</a> is set to the value of the end time divided by 100.		
	Reactor Models	• Closed Homogeneous Batch Reactor  • Closed Plasma Reactor  • IC HCCI Engine  • Non-reactive Gas Mixer  • Perfectly Stirred Reactor (PSR)  • Plasma PSR  • SI Engine Zonal Simulator		
	Notes	• See also: <a href="#">DELT</a> and <a href="#">DTSV</a> keywords.		
STST Reactor Property	The solution will be obtained using a steady-state calculation (with the solver <i>Twopnt</i> ) rather than a transient calculation (using the solver <i>DASPK</i> ).			
	Keyword Usage	Optional keyword. By default, a steady-state calculation is performed.		

Keyword	Definition			
	<b>Reactor Models</b>	<ul style="list-style-type: none"><li>• Non-reactive Gas Mixer</li><li>• Perfectly Stirred Reactor (PSR)</li><li>• Plasma PSR</li><li>• Rotating Disk CVD Reactor</li><li>• Stagnation Flow CVD Reactor</li></ul>		
	<b>Notes</b>	<ul style="list-style-type: none"><li>• Exclusive toggle with <a href="#">TRAN</a>.</li></ul>		
<b>SURF</b>  Reactor Property	Initial values (transient) or estimates (steady-state) for the surface site fraction values for the surface species on each surface site type (surface phase).			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Surface species name</i>	Required	--	SURF <b>Ga(s)</b> 0.001
	<i>Surface fractions</i>	Required	site fractions	SURF Ga(s) <b>0.001</b>
	<b>Keyword Usage</b>	Optional keyword. By default, the initial or estimated surface-site fractions are 0.0.		
	<b>Reactor Models</b>	<ul style="list-style-type: none"><li>• Closed Homogeneous Batch Reactor</li><li>• Closed Plasma Reactor</li><li>• Cylindrical Shear Flow Reactor</li><li>• Honeycomb Reactor</li><li>• Perfectly Stirred Reactor (PSR)</li><li>• Planar Shear Flow Reactor</li><li>• Plasma Plug Flow Reactor</li><li>• Plasma PSR</li><li>• Plug Flow Reactor</li><li>• Rotating Disk CVD Reactor</li><li>• Stagnation Flow CVD Reactor</li></ul>		
	<b>Notes</b>	<ul style="list-style-type: none"><li>• The sum of the site fractions should equal one for each surface site type (phase). However, if they do not, a cautionary message will be printed and the site fractions for each surface site type will be normalized so the sum does equal one.</li></ul>		
<b>SVSO</b>	Specify the reference gas viscosity at the reference temperature of the Sutherland's-law for viscosity.			

Keyword	Definition			
Reactor Property	Parameters	Optional/Reqd.	Units	Examples
	Reference gas viscosity at reference temperature	Required.	g/cm-s	SVS0 <b>1.716E-4</b>
	Keyword Usage	Optional.		
	Reactor Models	<ul style="list-style-type: none"><li>Multi-Zone HCCI Simulator</li><li>IC HCCI Engine</li><li>SI Engine Zonal Simulator</li></ul>		
SVSS	Specify the Sutherland temperature of the Sutherland's-law for viscosity.			
Reactor Property	Parameters	Optional/Reqd.	Units	Examples
	Sutherland temperature	Required.	K	SVSS <b>114.0</b>
	Keyword Usage	Optional.		
	Reactor Models	<ul style="list-style-type: none"><li>Multi-Zone HCCI Simulator</li><li>IC HCCI Engine</li><li>SI Engine Zonal Simulator</li></ul>		
SVST	Specify the reference temperature of the Sutherland's-law for viscosity.			
Reactor Property	Parameters	Optional/Reqd.	Units	Examples
	Reference temperature	Required.	K	SVST <b>273.15</b>
	Keyword Usage	Optional.		
	Reactor Models	<ul style="list-style-type: none"><li>Multi-Zone HCCI Simulator</li><li>IC HCCI Engine</li><li>SI Engine Zonal Simulator</li></ul>		
SYMT	Keyword for temperature boundary condition on the upper wall (only used for non-symmetric cartesian coordinates). The upper wall temperature is set equal to the bottom wall temperature if SYMT is specified.			
Reactor Property	Keyword Usage	Optional keyword. By default, an adiabatic top wall is used.		
	Reactor Models	<ul style="list-style-type: none"><li>Planar Shear Flow Reactor</li></ul>		

## 10.4. Alphabetical Listing of Keywords [T-Z]

**Table 10.4: Alphabetical Listing of Keywords [T-Z]**

Keyword	Definition			
<b>T1</b>  Reactor Property	Temperature before the incident shock.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Temperature</i>	Required	K	T1 <b>300.</b>
	<b>Keyword Usage</b>	Optional keyword. The shock velocity and any two of temperature, pressure, or density must be specified for conditions before the incident shock. See also <a href="#">P1A</a> and <a href="#">RHO1</a> .		
	<b>Reactor Models</b>	<ul style="list-style-type: none"><li>• Normal Incident Shock</li><li>• Normal Reflected Shock</li></ul>		
<b>T2</b>  Reactor Property	Temperature after the incident shock.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Temperature</i>	Required	K	T2 <b>1500.</b>
	<b>Keyword Usage</b>	Optional keyword. Any two of temperature, pressure, or density must be specified for conditions after the incident shock. See also <a href="#">RHO2</a> and <a href="#">P2A</a> .		
	<b>Reactor Models</b>	<ul style="list-style-type: none"><li>• Normal Incident Shock</li><li>• Normal Reflected Shock</li></ul>		
<b>T3</b>  Reactor Property	Temperature after the reflected shock, given as $T_5$ in the equations.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Temperature</i>	Required	K	T2 <b>1500.</b>
	<b>Keyword Usage</b>	Optional keyword. Any two of temperature, pressure, or density must be specified for conditions after the reflected shock. See also <a href="#">RHO3</a> and <a href="#">P3A</a> .		
	<b>Reactor Models</b>	<ul style="list-style-type: none"><li>• Normal Reflected Shock</li></ul>		
<b>TAMB</b>  Reactor Property	Ambient temperature for convective or conductive heat transfer out of the system. This keyword is only relevant when the energy equation is being solved.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Material name</i>	<b>Option- al.</b> If no material is specified, the same value will be used for all materials.	--	TAMB <b>material1</b> 298

Keyword	Definition			
	<i>Ambient temperature</i>	Required	K	TAMB <b>298</b>
	<i>Reactor number (PSR clusters only)</i>	<b>Optional.</b> If no number is given, the keyword is assumed to apply to all reactors in a cluster.	--	TAMB material1 298 <b>1</b>
	<b>Keyword Usage</b>	Optional keyword. This keyword must be used with <a href="#">HTC</a> .		
	<b>Reactor Models</b>	<ul style="list-style-type: none"> <li>• Closed Homogeneous Batch Reactor</li> <li>• Closed Plasma Reactor</li> <li>• Honeycomb Monolith Reactor</li> <li>• Non-reactive Gas Mixer</li> <li>• Perfectly Stirred Reactor (PSR)</li> <li>• Plasma PSR</li> <li>• Plasma Plug Flow Reactor</li> <li>• Plug Flow Reactor</li> </ul>		
Reactor Property	<b>TAU</b>	The nominal residence time of the gas in the reactor when flow is present.		
	Parameters	Optional/Reqd.	Units	Examples
	<i>Nominal residence time</i>	Required	sec	TAU <b>1.E-3</b>
	<i>Reactor number (PSR clusters only)</i>	Optional  If no number is given, the keyword is assumed to apply to all reactors	--	TAU 1.E-3 <b>1</b>



Keyword	Definition			
		in a cluster.		
	Keyword usage	PSRs: Optional keyword. If none of <a href="#">TAU</a> , <a href="#">FLRT</a> / <a href="#">FPRO</a> , <a href="#">SCCM</a> / <a href="#">SCCMPRO</a> are specified or are nonzero, then a closed-system is assumed. <a href="#">FLRT</a> / <a href="#">FPRO</a> or <a href="#">SCCM</a> / <a href="#">SCCMPRO</a> is required for each <a href="#">INLET</a> stream defined. PaSRs: Optional keyword. Unless the <a href="#">CLSE</a> keyword is used, any two of <a href="#">FLRT</a> , <a href="#">STPT</a> and reactor volume ( <a href="#">VOL</a> ) are required.		
	Reactor Models	<ul style="list-style-type: none"><li>Partially Stirred Reactor (PaSR)</li><li>Perfectly Stirred Reactor (PSR)</li><li>Plasma PSR</li></ul>		
TBND Solver	The upper boundary for gas temperature. Setting <a href="#">TBND</a> to the upper limit of thermodynamic data can prevent the <i>Gas-phase Kinetics</i> Pre-processor from getting erratic thermal data by extrapolating the fitting polynomials.			
	Parameters	Optional/Reqd.	Units	Examples
	Upper boundary	Required	K	TBND 10000.
	Keyword Usage	Optional keyword. By default, the upper boundary is 5000.		
	Reactor Models	<ul style="list-style-type: none"><li>Closed Homogeneous Batch Reactor</li><li>Closed Plasma Reactor</li><li>Diffusion of Premixed Opposed-flow Flame</li><li>Honeycomb Reactor</li><li>Perfectly Stirred Reactor (PSR)</li><li>Plasma Plug Flow Reactor</li><li>Plasma PSR</li><li>Plug Flow Reactor</li><li>Premixed Laminar Burner-stabilized Flame</li><li>Premixed Laminar Flame-speed Calculation</li><li>Rotating Disk CVD Reactor</li><li>Stagnation Flow CVD Reactor</li></ul>		
TBTH Reactor Property	Set the bath gas temperature in Kelvin. This temperature is used wherever a single temperature is needed. The default is 298.15 K.			
	Parameters	Optional/Reqd.	Units	Examples

Keyword	Definition			
	<i>Bath gas temperature</i>	Required	K	TBTH <b>900</b> .
	<b>Keyword Usage</b>	Optional keyword. By default, the bath gas temperature is 298.15.		
	<b>Reactor Models</b>	• Mechanism Analyzer		
<b>TDIF</b>	Include thermal diffusion (Soret effect) in the transport calculations.			
Reactor Property	<b>Keyword Usage</b>	Optional keyword. By default, thermal diffusion is not included.		
	<b>Reactor Models</b>	• Cylindrical Shear Flow Reactor  • Diffusion or Premixed Opposed-flow Flame  • Planar Shear Flow Reactor  • Premixed Laminar Burner-stabilized Flame  • Premixed Laminar Flame-speed Calculation  • Rotating Disk CVD Reactor  • Stagnation Flow CVD Reactor		
<b>TDEL</b>	Set the temperature increment in all tables where the temperature is varied.			
Reactor Property	Parameters	Optional/Reqd.	Units	Examples
	<i>Temperature</i>	Required	K	TDEL <b>200</b> .
	<b>Keyword Usage</b>	Optional keyword. By default, the temperature step is 100 K.		
	<b>Reactor Models</b>	• Mechanism Analyzer		
<b>TDSK</b>	Temperature of the deposition surface. This is a constant value taken as a boundary condition, unless the keyword <b>RADB</b> is given, indicating that the susceptor or disk temperature is calculated from an energy balance. If <b>RADB</b> is specified, <b>TDSK</b> is taken as the initial guess for the susceptor temperature.			
Reactor Property	Parameters	Optional/Reqd.	Units	Examples
	<i>Surface temperature</i>	Required	K	TDSK <b>1200</b>
	<b>Keyword Usage</b>	Required keyword.		
	<b>Reactor Models</b>	• Rotating Disk CVD Reactor  • Stagnation Flow CVD Reactor		
<b>TEBND</b>	The upper boundary for electron temperature. Can be useful for preventing non-plasma solutions in steady state problems.			
Reactor Property	Parameters	Optional/Reqd.	Units	Examples
	<i>Upper boundary</i>	Required	K	TEBND <b>8000</b>

Keyword	Definition			
	<b>Keyword Usage</b>	Optional keyword. By default, the upper boundary is 200000 K (roughly 20 eV).		
	<b>Reactor Models</b>	<ul style="list-style-type: none"><li>• Closed Plasma Reactor</li><li>• Plasma PSR</li><li>• Plasma Plug Flow Reactor</li></ul>		
<b>TEIN</b> Inlet Property	Electron temperature in the inlet stream. For most cases, there are no free electrons in the inlet stream, in which case the electron inlet temperature is not used.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Electron temperature</i>	Required	K	TEIN <b>300.</b>
	<b>Keyword Usage</b>	Optional keyword. By default, the electrons have the same temperature as the inlet gas.		
	<b>Reactor Models</b>	<ul style="list-style-type: none"><li>• Plasma PSR</li></ul>		
<b>TEMP</b> Reactor Property	The reactor gas temperature. Depending on the Reactor Model and problem type, this is either the user-supplied temperature constraint ( <a href="#">TGIV</a> ), an initial estimate of the temperature ( <a href="#">ENRG</a> ), or the initial reactor temperature (for transient cases). See also <a href="#">TPRO</a> .			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Reactor gas temperature</i>	Required	K	TEMP <b>1000.</b>
	<i>Reactor number (PSR clusters only)</i>	Optional If no number is given, the keyword is assumed to apply to all reactors in a cluster.	--	TEMP 1000. <b>1</b>
	<b>Keyword Usage</b>	Required keyword.		
	<b>Reactor Models</b>	<ul style="list-style-type: none"><li>• Chemical and Phase Equilibrium Calculations</li><li>• Closed Homogeneous Batch Reactor</li><li>• Closed Partially Stirred Reactor (PaSR)</li><li>• Closed Plasma Reactor</li><li>• Diffusion or Premixed Opposed-flow Flame</li></ul>		

Keyword	Definition			
		<ul style="list-style-type: none"><li>• Honeycomb Reactor</li><li>• IC HCCI Engine</li><li>• Non-reactive Gas Mixer</li><li>• Partially Stirred Reactor (PaSR)</li><li>• Perfectly Stirred Reactor (PSR)</li><li>• Plasma Plug Flow Reactor</li><li>• Plasma PSR</li><li>• Plug Flow Reactor</li><li>• Premixed Laminar Burner-stabilized Flame</li><li>• Premixed Laminar Flame-speed Calculation</li><li>• Rotating Disk CVD Reactor</li><li>• SI Engine Zonal Simulator</li><li>• Stagnation Flow CVD Reactor</li></ul>		
	Notes	<ul style="list-style-type: none"><li>• In previous versions, <b>TINI</b> keyword was used for some Reactor Models.</li></ul>		
TEST	Specifies an estimate of the equilibrium temperature.			
Reactor Property	Parameters	Optional/Reqd.	Units	Examples
	Temperature	Required	K	TEST <b>2000</b>
	Keyword Usage	Optional keyword. May help convergence to the equilibrium temperature, or assure an appropriate equilibrium temperature is calculated when a second, trivial solution exists (e.g., for adiabatic flame-temperature calculations).		
	Reactor Models	<ul style="list-style-type: none"><li>• Chemical and Phase Equilibrium Calculations</li></ul>		
TEXP	Specifies the average/cylinder temperature that defines the start of the expansion period. This keyword has a lower priority than <a href="#">QEXP</a> .			
Reactor Property	Parameters	Optional/Reqd.	Units	Examples
	temperature	Required	K	TEXP <b>1150.0</b>
	Keyword Usage	Optional keyword. Default = 1000K.		
	Reactor Models	<ul style="list-style-type: none"><li>• Multi-Zone HCCI Simulator</li><li>• IC HCCI Engine</li><li>• SI Engine Zonal Simulator</li></ul>		

Keyword	Definition			
TFAL  Output	Analyze the fall-off of a gas-phase reaction with respect to changes in the temperature, i.e., create a table of reaction rates versus temperature at a constant pressure. The pressure and gas composition are assumed to be that of the bath gas. The <b>ALL</b> option is the default and produces tables for every gas-phase reaction. The <b>NONE</b> option suppresses output for all of the reactions. If reaction information is desired for only certain reactions, they may be optionally specified by their number (given in the Pre-processor output) or by typing an exact duplicate of the reaction expression (see example input).			
	Parameters	Optional/Reqd.	Units	Examples
	<i>ALL option</i>	<b>Option- al, de- fault is ALL</b>	--	TFAL <b>ALL</b>
	<i>NONE option</i>	<b>Option- al, de- fault is ALL</b>	--	TFAL <b>NONE</b>
	<i>Gas reaction number list</i>	<b>Option- al, de- fault is ALL</b>	--	TFAL <b>2 5</b>
	<i>Gas reaction expression</i>	<b>Option- al, de- fault is ALL</b>	--	TFAL <b>2CH3(+M)&lt;=&gt;C2H6(+M)</b>
	<b>Keyword Usage</b>	Optional keyword. By default, the table output is determined by the <b>ALL</b> or <b>NONE</b> keyword.		
	<b>Reactor Models</b>	• Mechanism Analyzer		
TFIX  Reactor Property	When solving a freely propagating adiabatic flame ( <b>FREE</b> ), the problem is posed in a flame-fixed coordinate system. In this case the flame speed becomes an eigenvalue. Therefore, an additional constraint is required. We choose to supply this additional condition by fixing the temperature at one point in the flame, and this input allows the specification of that fixed temperature. Given the fixed temperature, the flame position is determined from the initial temperature profile as specified by the <b>TPRO</b> or <b>TPROF</b> inputs. If the fixed temperature is not one of the temperatures specified in the input, then a linear interpolation of the temperature profile to determine the position of <b>TFIX</b> is used and a mesh point added at that point.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Temperature</i>	<b>Option- al.</b>	K	TFIX <b>500.</b>
	<b>Keyword Usage</b>	Optional keyword. With <b>TPROF</b> , default is the average of unburned gas temperature ( <b>TUNBURNT</b> ) and mixture equilibrium temperature. With <b>TPRO</b> , the default is the average of the first and last Temperature profile values.		
	<b>Reactor Models</b>	• Premixed Laminar Flame-speed Calculation		

Keyword	Definition			
	Notes	• This keyword can be changed for a restart run.		
TGIV  Problem Type	Do not solve the gas energy equation, but will instead use a fixed user-supplied temperature (see <a href="#">TEMP</a> ).			
	Parameters	Optional/Reqd.	Units	Examples
	Reactor number (PSR clusters only)	Optional If no number is given, the keyword is assumed to apply to all reactors in a cluster.	--	TGIV <b>2</b>
	Keyword Usage	Optional keyword. Either <a href="#">TGIV</a> or <a href="#">ENRG</a> must be specified, unless <a href="#">CONP</a> , <a href="#">CONV</a> , or <a href="#">COTV</a> problem-types are specified for a closed system.		
	Reactor Models	<ul style="list-style-type: none"><li>• Closed Homogeneous Batch Reactor</li><li>• Closed Plasma Reactor</li><li>• Diffusion or Premixed Opposed-flow Flame</li><li>• Non-reactive Gas Mixer</li><li>• Honeycomb Reactor</li><li>• Perfectly Stirred Reactor (PSR)</li><li>• Plasma Plug Flow Reactor</li><li>• Plasma PSR</li><li>• Plug Flow Reactor</li><li>• Premixed Laminar Burner-stabilized Flame</li><li>• Rotating Disk CVD Reactor</li><li>• Stagnation Flow CVD Reactor</li></ul>		
	Notes	• This keyword can be removed or added for a restart run.		
THIG  Reactor Property	Set the upper limit of the temperature range (K) in all tables where the temperature is varied. The default is 1500 K.			
	Parameters	Optional/Reqd.	Units	Examples

Keyword	Definition			
	Temperature	Required	K	THIG <b>298.15</b>
	Keyword Usage	Optional keyword. By default, the high temperature is 1500.		
	Reactor Models	• Mechanism Analyzer		
THRM Output	Prints out individual thermodynamics tables for the species in the mechanism. The default is <b>ALL</b> , which generates the tables for all species in the mechanism. The GAS, SUR, and BULK options will cause thermodynamic tables for only species in the specified phase to be printed. Listing individual species by their name or by their number (as listed in the <i>Gas-phase Kinetics</i> or <i>Surface Kinetics</i> Pre-processor output files) will generate thermodynamic tables for the specified species. The keyword <b>NONE</b> will suppress all of the species thermodynamic tables.			
	Parameters	Optional/Reqd.	Units	Examples
	ALL option	Optional	--	THRM <b>ALL</b>
	NONE option	Optional	--	THRM <b>NONE</b>
	GAS option	Optional	--	THRM <b>GAS</b>
	SUR option	Optional	--	THRM <b>SUR</b>
	BULK option	Optional	--	THRM <b>BULK</b>
	Species name	Optional	--	THRM <b>CH4</b>
	Species number	Optional	--	THRM <b>3</b>
	Keyword Usage	Optional keyword. By default, the table output is determined by the <b>ALL</b> or <b>NONE</b> keyword.		
	Reactor Models	• Mechanism Analyzer		
TIFP Output	Calculate the ignition delay as the time when the slope of the temperature profile reaches its maximum value. You need to use sufficient number of time points to obtain an accurate temperature profile. Only applicable when you are solving the energy equation with the transient solver.			
	Keyword Usage	Optional keyword. See also <b>TLIM</b> and <b>DTIGN</b> .		
	Reactor Models	• Closed Homogeneous Batch Reactor  • Closed Plasma Reactor  • Honeycomb Monolith Reactor  • -IC HCCI Engine  • Perfectly Stirred Reactor (PSR)  • Plasma PSR  • Plasma Plug Flow Reactor  • Plug Flow Reactor  • SI Engine Zonal Simulator		

Keyword	Definition			
TIM1 Solver	For the steady-state solver, <i>Twopnt</i> , if the Newton method fails to converge, then the application takes some pseudo time steps in order to bring the current iterate within the domain of convergence of Newton's method. This input specifies how many time steps to take and the initial size of the time step, for the initial fixed-temperature calculation.			
	Parameters	Optional/Reqd.	Units	Examples
	Number of time steps	Required	--	TIM1 <b>50</b> 3.E-7
	Initial size of time step	Required	sec	TIM1 50 <b>3.E-7</b>
	Keyword Usage	Optional keyword. By default, the number of time steps is 100 and the initial size of the time step is 1.E-6. See also <a href="#">TIM2</a> .		
	Reactor Models	<ul style="list-style-type: none"><li>• Diffusion or Premixed Opposed-flow Flame</li><li>• Non-reactive Gas Mixer</li><li>• Perfectly Stirred Reactor (PSR)</li><li>• Plasma PSR</li><li>• Premixed Laminar Burner-stabilized Flame</li><li>• Premixed Laminar Flame-speed Calculation</li><li>• Rotating Disk CVD Reactor</li><li>• Stagnation Flow CVD Reactor</li></ul>		
	Notes	<ul style="list-style-type: none"><li>• In previous versions, <a href="#">TIME</a> keyword was used.</li></ul>		
TIM2 Solver	For the steady-state solver, <i>Twopnt</i> , if the Newton method fails to converge, then the application takes some pseudo time steps in order to bring the current iterate within the domain of convergence of Newton's method. This input specifies how many time steps to take and the initial size of the time step, when the energy equation is being solved.			
	Parameters	Optional/Reqd.	Units	Examples
	Number of time steps	Required	--	TIM2 <b>50</b> 3.E-7
	Initial size of time step	Required	sec	TIM2 50 <b>3.E-7</b>
	Keyword Usage	Optional keyword. By default, the number of time steps is 100 and the initial size of the time step is 1.E-6. See also <a href="#">TIM1</a> .		
	Reactor Models	<ul style="list-style-type: none"><li>• Diffusion or Premixed Opposed-flow Flame</li><li>• Non-reactive Gas Mixer</li><li>• Perfectly Stirred Reactor (PSR)</li></ul>		



Keyword	Definition			
		<ul style="list-style-type: none"><li>• Plasma PSR</li><li>• Premixed Laminar Burner-stabilized Flame</li><li>• Premixed Laminar Flame-speed Calculation</li><li>• Rotating Disk CVD Reactor</li><li>• Stagnation Flow CVD Reactor</li></ul>		
	Notes	• This input is only used when ENRG or ENGE is included.		
TIME  Solver	The total integration time for the transient simulation. If the job is a continuation run and the keyword CNTT is specified, the final time value will be the starting time plus the value of TIME.			
	Parameters	Optional/Reqd.	Units	Examples
	Total integration time	Required	sec	TIME 1.0E-2
	Keyword Usage	Required keyword, except in case of IC HCCI Engine, where NREV can be specified instead.		
	Reactor Models	<ul style="list-style-type: none"><li>• Closed Homogeneous Batch Reactor</li><li>• Closed Partially Stirred Reactor (PaSR)</li><li>• Closed Plasma Reactor</li><li>• IC HCCI Engine</li><li>• Non-reactive Gas Mixer</li><li>• Normal Incident Shock</li><li>• Normal Reflected Shock</li><li>• Partially Stirred Reactor (PaSR)</li><li>• Perfectly Stirred Reactor (PSR)</li><li>• Plasma PSR</li><li>• Rotating Disk CVD Reactor</li><li>• SI Engine Zonal Simulator</li><li>• Stagnation Flow CVD Reactor</li></ul>		
	Notes	• See also CNTT keyword.		
TINF  Reactor Property	Ambient temperature of the external environment, used for certain heat-transfer options.			
	Parameters	Optional/Reqd.	Units	Examples

Keyword	Definition			
	<i>ambient temperature</i>	Required	K	TINF <b>500</b>
	<b>Keyword Usage</b>	Shear Flow Reactors: Optional keyword. Only used if <a href="#">HTRN</a> option is included. By default, the inlet gas temperature is used for the ambient temperature ( <a href="#">TINL</a> ). Premixed and Diffusion Flames: Optional keyword. Only used if the user subroutine <a href="#">QFUN</a> is enabled.		
	<b>Reactor Models</b>	<ul style="list-style-type: none"><li>• Cylindrical Shear Flow Reactor</li><li>• Diffusion or Premixed Opposed-flow Flame</li><li>• Planar Shear Flow Reactor</li><li>• Premixed Laminar Burner-stabilized Flame</li><li>• Premixed Laminar Flame-speed Calculation</li></ul>		
<b>TINL</b>	The inlet temperature for an inlet stream.			
Inlet Property	Parameters	Optional/Reqd.	Units	Examples
	<i>Inlet stream name (for PSRs and CVD Reactors only)</i>	Optional If there is no stream name than the inlet temperature applies to all streams.	--	TINL <b>secondary_air</b> 400
	<i>Inlet temperature</i>	Required	K	TINL <b>400</b>
	<b>Keyword Usage</b>	Required for each inlet stream when then energy equation will be solved.		
	<b>Reactor Models</b>	<ul style="list-style-type: none"><li>• Cylindrical Shear Flow Reactor</li><li>• Diffusion or Premixed Opposed-flow Flame</li><li>• Non-reactive Gas Mixer</li><li>• Partially Stirred Reactor (PaSR)</li><li>• Perfectly Stirred Reactor (PSR)</li><li>• Planar Shear Flow Reactor</li><li>• Plasma PSR</li><li>• Rotating Disk CVD Reactor</li></ul>		

Keyword	Definition			
		• Stagnation Flow CVD Reactor		
	Notes	• In previous versions, <b>TFUE</b> , <b>TOXI</b> , <b>TINF</b> , and <b>GTMP</b> keywords were used.		
TINL  Reactor Property	The temperature of the stagnation plane.			
	Parameters	Optional/Reqd.	Units	Examples
	Stagnation plane name	Optional  If there is no stream name than the inlet temperature applies to all streams.	--	TINL <b>StagPlane</b> 600
	Stagnation plane temperature	Required	K	TINL <b>600</b>
	Keyword Usage	Required for each stagnation plane when then energy equation will be solved.		
	Reactor Models	• Burner-stabilized Stagnation Flow Reactor		
TION  Reactor Property	Specified temperature of ions. In this version of the software, there is no separate energy balance that accounts for ion energy gain above the gas temperature. The ions may, however, be much hotter than the neutral species, and this is accounted here as an additional energy loss from the deposited power required to heat the ions to the assumed temperature.			
	Parameters	Optional/Reqd.	Units	Examples
	Specified temperature of ions	Required	K	TION <b>11500.</b>
	Reactor number (PSR clusters only)	Optional  If no number is given, the value is assumed to apply to all reactors in a cluster.	--	TION 11500. <b>1</b>
	Keyword Usage	Optional keyword. By default, the ions have the same temperature as the neutral gas.		

Keyword	Definition			
	<b>Reactor Models</b>	<ul style="list-style-type: none"><li>• Closed Plasma Reactor</li><li>• Plasma Plug Flow Reactor</li><li>• Plasma PSR</li></ul>		
<b>TJAC</b> Solver	For the steady-state solver <i>TwoPnt</i> , specifies the maximum number of Newton steps that can be taken in performing the pseudo time-stepping before a new Jacobian is evaluated. If TJAC=1, then a full Newton method will result.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Retirement age</i>	Required	--	TJAC <b>15</b>
	<b>Keyword Usage</b>	Optional keyword. By default, the retirement age is set at 20.		
	<b>Reactor Models</b>	<ul style="list-style-type: none"><li>• Cylindrical Shear Flow Reactor</li><li>• Diffusion or Premixed Opposed-flow Flame</li><li>• Non-reactive Gas Mixer</li><li>• Perfectly Stirred Reactor (PSR)</li><li>• Plasma PSR</li><li>• Planar Shear Flow Reactor</li><li>• Premixed Laminar Burner-stabilized Flame</li><li>• Premixed Laminar Flame-speed Calculation</li><li>• Rotating Disk CVD Reactor</li><li>• Stagnation Flow CVD Reactor</li></ul>		
<b>TLIM</b> Output	For all transient problems in which the temperature is allowed to vary, an “ignition time” is computed, which is defined as the time or distance when the temperature first reaches a value equal to <b>TLIM</b> .			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Ignition temperature</i>	Required	K	TLIM <b>500</b>
	<b>Keyword Usage</b>	Optional keyword. See also <b>DTIGN</b> .		
	<b>Reactor Models</b>	<ul style="list-style-type: none"><li>• Closed Homogeneous Batch Reactor</li><li>• Closed Plasma Reactor</li><li>• Honeycomb Monolith Reactor</li><li>• IC HCCI Engine</li><li>• Perfectly Stirred Reactor (PSR)</li></ul>		

Keyword	Definition			
		<ul style="list-style-type: none"><li>• Plasma PSR</li><li>• Plasma Plug Flow Reactor</li><li>• Plug Flow Reactor</li><li>• SI Engine Zonal Simulator</li></ul>		
<b>TLOW</b>  Reactor Property	Set the lower limit of the temperature range (K) in all tables where the temperature is varied. The default is 300 K.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Temperature</i>	Required	K	TLOW <b>100.</b>
	<b>Keyword Usage</b>	Optional keyword. By default, the low temperature is 300 K.		
	<b>Reactor Models</b>	<ul style="list-style-type: none"><li>• Mechanism Analyzer</li></ul>		
<b>TMAX</b>  Reactor Property	Maximum temperature for use with profiles defined by the <a href="#">LINE</a> or <a href="#">PLAT</a> options.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Maximum temperature</i>	Required	K	TMAX <b>2500.</b>
	<b>Keyword Usage</b>	Optional keyword. By default, the maximum temperature is set at 2200 K.		
	<b>Reactor Models</b>	<ul style="list-style-type: none"><li>• Diffusion or Premixed Opposed-flow Flame</li></ul>		
<b>TOFF</b>  Reactor Property	This keyword is used to tell the <i>TwoPnt</i> solver to ignore the temperature when adapting the grid. This can be useful for strained flames, since the temperature gradients can be very steep and, without this option, too many points will be placed in the same place without improving the solution. The flame can be well resolved by basing adaptation only on the species and velocity profiles.			
	<b>Keyword Usage</b>	Optional keyword. By default, the temperature is considered during adaptation.		
	<b>Reactor Models</b>	<ul style="list-style-type: none"><li>• Rotating Disk CVD Reactor</li><li>• Stagnation Flow CVD Reactor</li></ul>		
<b>TP</b>  Problem Type	Constant pressure and temperature constraint.			
	<b>Keyword Usage</b>	Optional keyword. Exactly one problem-type keyword must be included.		
	<b>Reactor Models</b>	<ul style="list-style-type: none"><li>• Chemical and Phase Equilibrium Calculations</li></ul>		
	<b>Notes</b>	<ul style="list-style-type: none"><li>• <b>PT</b> keyword is equivalent.</li></ul>		
<b>TPRO</b>  Reactor Property Profiles	Reactor gas temperature profile specified as a function of time for transient 0-D homogeneous systems or as a function of distance for channel-flow reactors or reactors where there is a constrained temperature. For 1-D steady-state Reactor Models where the energy equation is being solved, <a href="#">TPRO</a> is used to specify an initial temperature profile estimate.			

Keyword	Definition			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Time or Distance value, depending on Reactor Model</i>	Required	sec or cm	TPRO <b>1.0E-4</b> 1000
	<i>Gas Temperature</i>	Required	K	TPRO 1.0E-4 <b>1000</b>
	<i>Reactor number (PSR clusters only)</i>	Optional  If no number is given, the profile described by the first two values is assumed to apply to all reactors in a cluster.	--	TPRO 1.0E-4 1000 <b>1</b>
	<b>Keyword Usage</b>	Optional keyword. By default, no profile is provided.		
	<b>Reactor Models</b>	<ul style="list-style-type: none"> <li>• Closed Homogeneous Batch Reactor</li> <li>• Closed Plasma Reactor</li> <li>• Cylindrical Shear Flow Reactor</li> <li>• Diffusion or Premixed Opposed-flow Flame</li> <li>• Honeycomb Reactor</li> <li>• Non-reactive Gas Mixer</li> <li>• Perfectly Stirred Reactor (PSR)</li> <li>• Planar Shear Flow Reactor</li> <li>• Plasma Plug Flow Reactor</li> <li>• Plasma PSR</li> <li>• Plug Flow Reactor</li> <li>• Premixed Laminar Burner-stabilized Flame</li> <li>• Premixed Laminar Flame-speed Calculation</li> <li>• Rotating Disk CVD Reactor</li> <li>• Stagnation Flow CVD Reactor</li> </ul>		

Keyword	Definition			
TPROF  Reactor Property	Reactor gas temperature profile estimated as a function of distance for flame speed simulator and pre-mixed burner simulator with the energy equation being solved. It uses unburned gas temperature and mixture equilibrium temperature as corresponding upper and lower bounds. When TPROF is used, user-specified values of estimated center position (XCEN), estimated zone width (WMIX), and optional temperature constraint (TFIX) are ignored and pre-defined values are used. When TPROF is used with no NPTS, a default non-linear12-point grid is initialized, while TPROF with NPTS initializes a linear NPTS-point grid.			
	Keyword Usage	Optional keyword.		
	Reactor Models	<ul style="list-style-type: none"><li>Premixed Laminar Burner-stabilized Flame</li><li>Premixed Laminar Flame-speed Calculation</li></ul>		
TPRO-FILE_n  Reactor Property	Choice for the initial temperature profile. Integer n can be 1 or 2. Option 1 means a dumped energy profile (that is, all internal grid-points at specified maximum temperature) and option 2 means a linear profile from the boundary to grid-point where mixture fraction value is stoichiometric.			
	Keyword Usage	Required keyword. The default value is TPROFILE_1.		
	Reactor Models	<ul style="list-style-type: none"><li>Diffusion Flamelet Generator</li></ul>		
TRAD  Reactor Property	Temperature of a radiating disk located above and parallel to the substrate, used in calculating a surface radiation balance. A hot radiating disk may be included in addition to a cool “wall” ( TWAL), to represent, for example, a burner inlet. The geometry and location of the radiating disk are controlled by keywords RDSK and RRAD. TRAD is used only if the disk temperature is being calculated by including keyword RADB . See Equation 14.18 of the Chemkin-Pro Theory Manual .			
	Parameters	Optional/Reqd.	Units	Examples
	Temperature of a radiating disk	Required	K	TRAD 2500.
	Keyword Usage	Optional keyword. By default, the temperature of a radiating disk is 1000 K.		
	Reactor Models	<ul style="list-style-type: none"><li>Rotating Disk CVD Reactor</li><li>Stagnation Flow CVD Reactor</li></ul>		
TRAN  Solver	Perform a transient calculation instead of a steady-state calculation. For flame simulators, this input also specifies how many time steps to take and the initial size of the time step. Perform a transient calculation (with the solver DASPK) instead of a steady-state calculation (using the solver Twopnt).			
	Keyword Usage	Required keyword for Closed Homogeneous Batch Reactor, Closed Plasma Reactor, and the IC HCCI Engine. Otherwise, a steady-state calculation is performed by default.		
	Reactor Models	<ul style="list-style-type: none"><li>Closed Homogeneous Batch Reactor</li><li>Closed Plasma Reactor</li></ul>		

Keyword	Definition			
		<ul style="list-style-type: none"><li>• IC HCCI Engine</li><li>• Non-reactive Gas Mixer</li><li>• Perfectly Stirred Reactor (PSR)</li><li>• Plasma PSR</li><li>• Rotating Disk CVD Reactor</li><li>• Stagnation Flow CVD Reactor</li><li>• Diffusion or Premixed Opposed-flow Flame</li><li>• Premixed Laminar Burner-stabilized Flame</li><li>• Premixed Laminar Flame-speed Calculation</li><li>• SI Engine Zonal Simulator</li></ul>		
	Notes	<ul style="list-style-type: none"><li>• See also <a href="#">STST</a>.</li></ul>		
TRAN Output	Prints out the transport database properties (intermolecular potential parameters) for each gas-phase species in the mechanism. This feature also expands the thermo table to create a table of transport properties as a function of temperature. The <a href="#">NONE</a> option turns off printing of this table. The <i>Transport</i> Pre-processor must have been run successfully, unless the <a href="#">NONE</a> option is used.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>ALL option</i>	Optional	--	TRAN <b>ALL</b>
	<i>NONE option</i>	Optional	--	TRAN <b>NONE</b>
	Keyword Usage	Optional keyword. By default, the table output is determined by the <a href="#">ALL</a> or <a href="#">NONE</a> keyword.		
	Reactor Models	<ul style="list-style-type: none"><li>• Mechanism Analyzer</li></ul>		
TRCE Reactor Property	Including this keyword causes the calculation to be run by setting the mass fraction of the last-named <i>Gas-phase Kinetics</i> gas-phase species (or when <a href="#">REOR</a> is used, the species with the largest concentration) to be one minus the sum of the mass fractions of the other species. A conservation equation is not solved for the last (or largest-concentration) species.			
	Keyword Usage	Optional keyword. By default, correction velocity formalism is used.		
	Reactor Models	<ul style="list-style-type: none"><li>• Premixed Laminar Burner-stabilized Flame</li><li>• Premixed Laminar Flame-speed Calculation</li><li>• Rotating Disk CVD Reactor</li><li>• Stagnation Flow CVD Reactor</li></ul>		
	Notes	<ul style="list-style-type: none"><li>• This keyword can be removed or added for a restart run.</li></ul>		



Keyword	Definition			
TRES  Restart	Assigns a new initial time for a calculation that starts using the solution read from an XML Solution File.			
	Parameters	Optional/Reqd.	Units	Examples
	Initial time	Required	sec	TRES <b>0.0</b>
	Keyword Usage	Optional keyword. By default, the value of time found on the XML Solution File will be used.		
	Reactor Models	<ul style="list-style-type: none"><li>• Closed Homogeneous Batch Reactor</li><li>• Closed Partially Stirred Reactor (PaSR)</li><li>• Closed Plasma Reactor</li><li>• IC HCCI Engine</li><li>• Partially Stirred Reactor (PaSR)</li><li>• Perfectly Stirred Reactor (PSR)</li><li>• Plasma PSR</li><li>• SI Engine Zonal Simulator</li></ul>		
TRMAX-ITER  Solver	The maximum number of iterations time step in TWOPNT's time stepping algorithm. If TWOPNT exceeds this maximum, then it will cut its time step and try again. You may occasionally need to use this option is the time stepping algorithm is having difficulty solving your problem.			
	Parameters	Optional/Reqd.	Units	Examples
	Maximum iterations per time step	Optional	--	TRMAXITER <b>50</b>
	Keyword Usage	Optional keyword. By default, the maximum number of iterations is 25.		
	Reactor Models	<ul style="list-style-type: none"><li>• Cylindrical Shear Flow Reactor</li><li>• Diffusion or Premixed Opposed-flow Flame</li><li>• Non-reactive Gas Mixer</li><li>• Perfectly Stirred Reactor (PSR)</li><li>• Planar Shear Flow Reactor</li><li>• Plasma PSR</li><li>• Premixed Laminar Burner-stabilized Flame</li><li>• Premixed Laminar Flame-speed Calculation</li><li>• Rotating Disk CVD Reactor</li><li>• Stagnation Flow CVD Reactor</li></ul>		

Keyword	Definition			
	Notes	• TRMAXITER must be >=1.		
TRST Restart	Tells the application which time value in an XML Solution File to use for the initial conditions of the current calculation.			
	Parameters	Optional/Reqd.	Units	Examples
	Time value	Required	sec	TRST <b>1.0E-5</b>
	Keyword Usage	Optional keyword. By default, the last time value found on the XML Solution File will be used.		
	Reactor Models	<ul style="list-style-type: none"><li>• Closed Homogeneous Batch Reactor</li><li>• Closed Plasma Reactor</li><li>• Honeycomb Reactor</li><li>• IC HCCI Engine</li><li>• Perfectly Stirred Reactor (PSR)</li><li>• Plasma Plug Flow Reactor</li><li>• Plasma PSR</li><li>• Plug Flow Reactor</li><li>• SI Engine Zonal Simulator</li></ul>		
TS Problem Type	Constant entropy and temperature constraints.			
	Keyword Usage	Optional keyword. Exactly one problem-type keyword must be included.		
	Reactor Models	<ul style="list-style-type: none"><li>• Chemical and Phase Equilibrium Calculations</li></ul>		
	Notes	• <b>ST</b> keyword is equivalent.		
TSCCM Inlet Property	Sets the standard reference temperature used to define the flow rate when it is input in standard cubic centimeters per minute (sccm), i.e., when <b>SCCM</b> or <b>SCCMPRO</b> keywords are used.			
	Parameters	Optional/Reqd.	Units	Examples
	Standard temperature	Required	K	TSCCM <b>300</b>
	Keyword Usage	Optional keyword. By default, the reference temperature is set to 298.15 K.		
	Reactor Models	<ul style="list-style-type: none"><li>• Non-reactive Gas Mixer</li><li>• Perfectly Stirred Reactor (PSR)</li><li>• Plasma PSR</li><li>• Rotating Disk CVD Reactor</li></ul>		

Keyword	Definition			
		• Stagnation Flow CVD Reactor		
TS-FAC  Reactor Property/Model	The maximum liquid/droplet temperature allowed to prevent issues from liquid property evaluation. This maximum temperature value is specified as a fraction of the lowest critical temperature of the liquid component.			
	Parameters	Optional/Reqd.	Units	Examples
	Temperature change	Required	K	TSFAC <b>5.0</b>
	Keyword Usage	Optional keyword. Default is 1 K.		
	Reactor Models	• Direct Injection Diesel Engine Simulator		
TS-PL  Reactor Property Profiles	This keyword allows an optional specification of a spline-fit surface temperature profile of the lower wall for planar non-symmetric cases or otherwise the surface temperature profile of the upper wall. The data point describing the surface temperature profile is formatted as an $(x,T)$ pair. There is a <a href="#">TSPL</a> keyword line for each desired $(x,T)$ pair. The $x$ coordinates of each <a href="#">TSPL</a> line must be given in ascending order. A spline fit is used to interpolate between points.			
	Parameters	Optional/Reqd.	Units	Examples
	$x$ coordinate	Required	cm	TSPL <b>0.1</b> 973
	$T$ coordinate	Required	K	TSPL 0.1 <b>973</b>
	Keyword Usage	Optional keyword. By default, for symmetric cases default is specified constant temperature; for non-symmetric cases the wall is adiabatic.		
	Reactor Models	• Cylindrical Shear Flow Reactor  • Planar Shear Flow Reactor		
	Notes	• See also: <a href="#">TPRO</a> .		
	TS-RF  Reactor Property	The temperature of the surfaces in the reactor. Use only if you want the surface temperature, which controls the surface chemistry rates, to be different than the gas temperature.		
Parameters		Optional/Reqd.	Units	Examples
Material (for 0-D homogeneous and plug-flow reactors only)		Optional If not specified, then the temperature is the same for all materials.	--	TSRF <b>WAFER</b> 1200.
Surface temperature		Required	K	TSRF 1200.

Keyword	Definition			
	Reactor number (PSR clusters only)	Optional If no number is given, the value is assumed to apply to all reactors in a cluster.	--	TSRF 1200. <b>1</b>
	Keyword Usage	Closed Homogeneous, PSRs, and Plug Flow Reactors: Optional keyword. If not specified, the surface temperature is assumed to be the same as the gas temperature. Shear Flow Reactors: Required keyword.		
	Reactor Models	<ul style="list-style-type: none"><li>• Closed Homogeneous Batch Reactor</li><li>• Closed Plasma Reactor</li><li>• Cylindrical Shear Flow Reactor</li><li>• Diffusion or Premixed Opposed-flow Flame</li><li>• Honeycomb Reactor</li><li>• Perfectly Stirred Reactor (PSR)</li><li>• Planar Shear Flow Reactor</li><li>• Plasma Plug Flow Reactor</li><li>• Plasma PSR</li><li>• Plug Flow Reactor</li></ul>		
	Notes	<ul style="list-style-type: none"><li>• In previous versions, <b>STMP</b> keyword was used.</li></ul>		
TSTAU  Reactor Property/Model	An artificial damping factor to control how the droplet temperature approaches the maximum temperature value. A large damping factor will result in a smooth droplet temperature profile as it rises towards the maximum value. The damping factor value must be greater than 1K.			
	Parameters	Optional/Reqd.	Units	Examples
	Temperature change	Required	K	TSTAU <b>5.0</b>
	Keyword Usage	Optional keyword. Default is 1 K.		
	Reactor Models	<ul style="list-style-type: none"><li>• Direct Injection Diesel Engine Simulator</li></ul>		
TSTP	Initial time step used for integration of the fictitious transient equations used to determine an initial set of surface site fractions for the plug-flow simulation.			

Keyword	Definition			
Solver	Steady-state is assumed to be reached when there is no significant change in the surface site fractions over the course of one time step (see <a href="#">RCHG</a> ).			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Initial time step</i>	Required	cm	TSTP <b>0.1</b>
	<b>Keyword Usage</b>	Optional keyword. By default, the initial time step is 1.		
	<b>Reactor Models</b>	<ul style="list-style-type: none"><li>• Honeycomb Reactor</li><li>• Plasma Plug Flow Reactor</li><li>• Plug Flow Reactor</li></ul>		
TSTR Cluster Property	This keyword is valid when using the <a href="#">XMLI</a> , <a href="#">XMLS</a> or <a href="#">RSTR</a> option, when the XML Solution File used for initialization or restart contains transient data. In this case, select the values to use in initialization or restart as those corresponding to the time that is closest to (greater than or equal to) the specified time.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Time</i>	Required	sec	TSTR <b>0.01</b>
	<b>Keyword Usage</b>	Optional keyword. By default, uses the data from the last time-step found in the XML Solution File.		
	<b>Reactor Models</b>	<ul style="list-style-type: none"><li>• Chemical and Phase Equilibrium Calculations</li><li>• Closed Homogeneous Batch Reactor</li><li>• Closed Plasma Reactor</li><li>• Cylindrical Shear Flow Reactor</li><li>• Diffusion or Premixed Opposed-flow Flame</li><li>• Honeycomb Reactor</li><li>• IC HCCI Engine</li><li>• Mechanism Analyzer</li><li>• Non-reactive Gas Mixer</li><li>• Normal Incident Shock</li><li>• Normal Reflected Shock</li><li>• Perfectly Stirred Reactor (PSR)</li><li>• Planar Shear Flow Reactor</li><li>• Plasma Plug Flow Reactor</li><li>• Plasma PSR</li><li>• Plug Flow Reactor</li></ul>		

Keyword	Definition			
		<ul style="list-style-type: none"><li>• Premixed Laminar Burner-stabilized Flame</li><li>• Premixed Laminar Flame-speed Calculation</li><li>• Rotating Disk CVD Reactor</li><li>• SI Engine Zonal Simulator</li><li>• Stagnation Flow CVD Reactor</li></ul>		
<b>TSTR</b>  Solver	Starting time for the simulation.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Time</i>	Required	sec	TSTR <b>0.01</b>
	<b>Keyword Usage</b>	Optional keyword. By default, the starting time is 0.0		
	<b>Reactor Models</b>	<ul style="list-style-type: none"><li>• Normal Incident Shock</li><li>• Normal Reflected Shock</li></ul>		
<b>TSUM</b>  Output	Controls the printing of summary tables for the thermodynamic functions at the bath gas conditions (see <a href="#">TBTH</a> , <a href="#">PRES</a> , and <a href="#">XBTH</a> ). There are three sets of thermodynamic tables: one for the species, one for the gas reactions, and one for the surface reactions. The last three options turn on each table individually. The default is <a href="#">ALL</a> , which will print all three thermodynamic tables. They may all be suppressed with <a href="#">NONE</a> .			
	Parameters	Optional/Reqd.	Units	Examples
	<i>ALL option</i>	Optional	--	TSUM <b>ALL</b>
	<i>NONE option</i>	Optional	--	TSUM <b>NONE</b>
	<i>SPECIES option</i>	Optional	--	TSUM <b>SPECIES</b>
	<i>GAS option</i>	Optional	--	TSUM <b>GAS</b>
	<i>SUR option</i>	Optional	--	TSUM <b>SUR</b>
	<b>Keyword Usage</b>	Optional keyword. By default, the table output is determined by the <a href="#">ALL</a> or <a href="#">NONE</a> keyword.		
	<b>Reactor Models</b>	<ul style="list-style-type: none"><li>• Mechanism Analyzer</li></ul>		
<b>TSWH</b>  Reactor Property	Defines when the calculation will be switched from <a href="#">TGIV</a> to <a href="#">ENRG</a> with Woschni correlation as the heat transfer model. The default value is 0 sec (always use energy equation).			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Time in seconds</i>	Required	sec	TSWH 0.001
	<b>Keyword Usage</b>	Optional keyword.		
	<b>Reactor Models</b>	<ul style="list-style-type: none"><li>• Multi-Zone HCCI Engine Simulation</li></ul>		
<b>TTIM</b>  Reactor Property	The solution will be obtained with pressure and temperature given as specified functions of time through a user-programmed subroutine. The SUBROUTINE PSTEMPT (TIME, LOUT, TEMP, PA) must be provided to specify the temperature			

Keyword	Definition			
	and linked to the application program. See the Application Programming Interface Manual for information on how to work with user subroutines.			
	Keyword Usage	Optional keyword. By default, temperature and pressure will be specified by keyword. See also <a href="#">TPRO</a> and <a href="#">PPRO</a> .		
	Reactor Models	<ul style="list-style-type: none"><li>• Closed Homogeneous Batch Reactor</li><li>• Closed Plasma Reactor</li><li>• IC HCCI Engine</li><li>• Non-reactive Gas Mixer</li><li>• Perfectly Stirred Reactor (PSR)</li><li>• Plasma PSR</li><li>• SI Engine Zonal Simulator</li></ul>		
	Notes	<ul style="list-style-type: none"><li>• See also <a href="#">TPRO</a> and <a href="#">PPRO</a> as alternative ways to specify temperature and pressure as functions of time.</li></ul>		
TUN-BURNT	Unburned gas temperature.			
Reactor Property	Parameters	Optional/Reqd.	Units	Examples
	Unburned gas temperature	Required	K	TUNBURNT <b>300.0</b>
	Keyword Usage	Required keyword.		
	Reactor Models	<ul style="list-style-type: none"><li>• Premixed Laminar Burner-stabilized Flame</li><li>• Premixed Laminar Flame-speed Calculation</li></ul>		
TV	Constant volume and temperature constraints.			
Problem Type	Keyword Usage	Optional keyword. Exactly one problem-type keyword must be included.		
	Reactor Models	<ul style="list-style-type: none"><li>• Chemical and Phase Equilibrium Calculations</li></ul>		
	Notes	<ul style="list-style-type: none"><li>• <b>VT</b> keyword is equivalent.</li></ul>		
TWAB	Absolute error tolerance used by the steady-state <i>Twopnt</i> solver in the initial calculation at the inlet boundary.			
Solver	Parameters	Optional/Reqd.	Units	Examples
	Absolute error tolerance	Required	--	TWAB <b>1.0E-5</b>
	Keyword Usage	Optional keyword. By default, the absolute error tolerance is 1.0E-13.		
	Reactor Models	<ul style="list-style-type: none"><li>• Cylindrical Shear Flow Reactor</li><li>• Planar Shear Flow Reactor</li></ul>		

Keyword	Definition			
TW-AL  Reactor Property	Temperature of a neighboring “wall” used in calculating a surface radiation balance. This value is used only if the disk temperature is being calculated by including keyword RADB . See Equation 14.18 of the Chemkin-Pro Theory Manual .			
	Parameters	Optional/Reqd.	Units	Examples
	Wall temperature	Required	K	TWAL <b>850.0</b>
	Keyword Usage	Optional keyword. By default, the wall temperature is 500 K.		
	Reactor Models	<ul style="list-style-type: none"><li>Rotating Disk CVD Reactor</li><li>Stagnation Flow CVD Reactor</li></ul>		
TW-PR  Output	Specifies print level for the initial steady-state solution of the inlet boundary by the Twopnt solver.			
	Parameters	Optional/Reqd.	Units	Examples
	Print level	Required	--	TWPR <b>0</b>
	Keyword Usage	Optional keyword. By default, the print level is set at 22.		
	Reactor Models	<ul style="list-style-type: none"><li>Cylindrical Shear Flow Reactor</li><li>Planar Shear Flow Reactor</li></ul>		
TWRE  Solver	Relative error tolerance used by the steady-state Twopnt solver in the initial calculation at the inlet boundary.			
	Parameters	Optional/Reqd.	Units	Examples
	Relative error tolerance	Required	--	TWRE <b>1.0E-10</b>
	Keyword Usage	Optional keyword. By default, the relative error tolerance is 1.0E-4.		
	Reactor Models	<ul style="list-style-type: none"><li>Cylindrical Shear Flow Reactor</li><li>Planar Shear Flow Reactor</li></ul>		
TWST  Solver	Number of time steps before trying another Newton step, used by the steady-state Twopnt solver in the initial calculation at the inlet boundary.			
	Parameters	Optional/Reqd.	Units	Examples
	Number of time steps	Required	--	TWST <b>50</b>
	Keyword Usage	Optional keyword. By default, the number of time steps is set at 100.		
	Reactor Models	<ul style="list-style-type: none"><li>Cylindrical Shear Flow Reactor</li><li>Planar Shear Flow Reactor</li></ul>		



Keyword	Definition			
UFAC Solver	Factor by which to multiply the time step in the steady-state <i>TwoPnt</i> 's pseudo time stepping procedure when the number of time steps at the current step size reaches the number specified by <i>IRET</i> .			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Multiply factor</i>	Required	--	UFAC <b>2.2</b>
	<b>Keyword Usage</b>	Optional keyword. By default, the multiplication factor is set to 2.0.		
	<b>Reactor Models</b>	<ul style="list-style-type: none"><li>• Diffusion or Premixed Opposed-flow Flame</li><li>• Non-reactive Gas Mixer</li><li>• Perfectly Stirred Reactor (PSR)</li><li>• Plasma PSR</li><li>• Rotating Disk CVD Reactor</li><li>• Stagnation Flow CVD Reactor</li></ul>		
UIGN Output, User Subroutine	Use the ignition delay time definition given in the user routine <i>PSIGNT</i> . Only applicable when you are solving the energy equation with transient solver. See the Application Programming Interface Manual for details on how to work with user subroutines.			
	Parameters	Optional/Reqd.	Units	Examples
	<b>Keyword Usage</b>	Optional keyword.		
	<b>Reactor Models</b>	<ul style="list-style-type: none"><li>• Closed Homogeneous Batch Reactor</li><li>• Closed Plasma Reactor</li><li>• Honeycomb Monolith Reactor</li><li>• IC HCCI Engine</li><li>• Perfectly Stirred Reactor (PSR)</li><li>• Plasma PSR</li><li>• Plasma Plug Flow Reactor</li><li>• Plug Flow Reactor</li><li>• SI Engine Zonal Simulator</li></ul>		
	UINL Reactor Property	The axial velocity at the inlet boundary. If the rotations rate <i>OMEG</i> is zero, or if the <i>STAG</i> option is used, then <i>UINL</i> is no longer optional, but must be given to specify the problem.		
Parameters		Optional/Reqd.	Units	Examples
<i>Axial inlet velocity</i>		Required	cm/sec	UINL <b>23.6</b>

Keyword	Definition	
	<b>Keyword Usage</b>	Diffusion or Premixed Opposed-flow Flames: Required keyword for each inlet stream. Rotating Disk CVD Reactor: Optional keyword. The velocity at the outer domain is calculated as a part of the solution. However, using the keyword <a href="#">UINL</a> , one may impose this velocity upon the solution. By default, the axial inlet velocity is 0. Stagnation Flow CVD Reactor: Required keyword.
	<b>Reactor Models</b>	<ul style="list-style-type: none"> <li>• Diffusion or Premixed Opposed-flow Flame</li> <li>• Rotating Disk CVD Reactor</li> <li>• Stagnation Flow CVD Reactor</li> </ul>
	<b>Notes</b>	<ul style="list-style-type: none"> <li>• In previous versions: <b>UINF</b>, <b>VFUE</b>, or <b>VOXI</b> keywords were used.</li> </ul>
<b>UP-ROF</b>	Reactor inlet profiles will be given by a user-programmed subroutine. SUBROUTINE CRUPROF must be provided to specify the inlet profiles of all variables and linked to the application program. See the Application Programming Interface Manual for details on how to work with user subroutines.	
Reactor Property, User Subroutine	<b>Keyword Usage</b>	Optional keyword. By default, a uniform inlet profile is used for all variables except axial velocity. The axial velocity profile is uniform in the Planar Shear Flow Reactor model and is parabolic (or fully developed) in the Cylindrical Shear Flow Reactor model.
	<b>Reactor Models</b>	<ul style="list-style-type: none"> <li>• Cylindrical Shear Flow Reactor</li> <li>• Planar Shear Flow Reactor</li> </ul>
<b>UREF</b>	For the IC HCCI Engine ( <a href="#">ICEN</a> ), the heat transfer model ( <a href="#">ICHT</a> ) evaluates viscosity and thermal conductivity using the instantaneous temperature and pressure inside the cylinder. The <a href="#">UREF</a> keyword is a flag that instructs the heat transfer model to use transport properties evaluated at the initial condition instead. <a href="#">UREF</a> is turned off by default therefore it must be added to old input files in which keyword <a href="#">ICHT</a> is used to reproduce the old results.	
Reactor Property	<b>Keyword Usage</b>	Optional keyword. By default, properties are evaluated using local conditions.
	<b>Reactor Models</b>	<ul style="list-style-type: none"> <li>• IC HCCI Engine</li> <li>• SI Engine Zonal Simulator</li> </ul>
<b>USE</b>	Uses an initial non-uniform grid based on points specified in the estimated temperature profile (TPRO or TPROF).	
<a href="#">_TPRO_GRID</a>	<b>Keyword Usage</b>	Optional keyword.
Reactor Property	<b>Reactor Models</b>	<ul style="list-style-type: none"> <li>• Premixed Laminar Burner-Stabilized Flame</li> <li>• Premixed Laminar Flame-Speed Calculation</li> </ul>

Keyword	Definition	
<b>USEP</b>  Cluster Property	For use with XMLI, XMLS, or RSTR, to override the values of pressure found on the XML Solution File used for restart or initialization with those specified in the user input file.	
	<b>Keyword Usage</b>	Optional keyword. By default, the program uses the pressure from the XML Solution File.
	<b>Reactor Models</b>	<ul style="list-style-type: none"> <li>• Chemical and Phase Equilibrium Calculations</li> <li>• Closed Homogeneous Batch Reactor</li> <li>• Closed Plasma Reactor</li> <li>• Cylindrical Shear Flow Reactor</li> <li>• Diffusion or Premixed Opposed-flow Flame</li> <li>• Honeycomb Reactor</li> <li>• IC HCCI Engine</li> <li>• Mechanism Analyzer</li> <li>• Non-reactive Gas Mixer</li> <li>• Normal Incident Shock</li> <li>• Normal Reflected Shock</li> <li>• Perfectly Stirred Reactor (PSR)</li> <li>• Planar Shear Flow Reactor</li> <li>• Plasma Plug Flow Reactor</li> <li>• Plasma PSR</li> <li>• Plug Flow Reactor</li> <li>• Premixed Laminar Burner-stabilized Flame</li> <li>• Premixed Laminar Flame-speed Calculation</li> <li>• Rotating Disk CVD Reactor</li> <li>• Stagnation Flow CVD Reactor</li> </ul>
<b>USET</b>  Cluster Property	For use with XMLI, XMLS, or RSTR, override the values of temperature found on the XML Solution File used for restart or initialization with those specified in the user input file.	
	<b>Keyword Usage</b>	Optional keyword. By default, the program uses the temperature from the XML Solution File.
	<b>Reactor Models</b>	<ul style="list-style-type: none"> <li>• Chemical and Phase Equilibrium Calculations</li> <li>• Closed Homogeneous Batch Reactor</li> </ul>

Keyword	Definition	
		<ul style="list-style-type: none"> <li>• Closed Plasma Reactor</li> <li>• Cylindrical Shear Flow Reactor</li> <li>• Diffusion or Premixed Opposed-flow Flame</li> <li>• Honeycomb Reactor</li> <li>• IC HCCI Engine</li> <li>• Mechanism Analyzer</li> <li>• Non-reactive Gas Mixer</li> <li>• Normal Incident Shock</li> <li>• Normal Reflected Shock</li> <li>• Perfectly Stirred Reactor (PSR)</li> <li>• Planar Shear Flow Reactor</li> <li>• Plasma Plug Flow Reactor</li> <li>• Plasma PSR</li> <li>• Plug Flow Reactor</li> <li>• Premixed Laminar Burner-stabilized Flame</li> <li>• Premixed Laminar Flame-speed Calculation</li> <li>• Rotating Disk CVD Reactor</li> <li>• SI Engine Zonal Simulator</li> <li>• Stagnation Flow CVD Reactor</li> </ul>
	<b>Notes</b>	<ul style="list-style-type: none"> <li>• In previous versions, <b>USTG</b> keyword was used.</li> </ul>
<b>USEV</b>  Restart	This keyword is valid when using <b>XMLI</b> or the <b>RSTR</b> options. When this keyword is included, it overrides the values of velocity or flow-rate found on the XML Solution File used for restart or initialization with those specified in the user input file.	
	<b>Keyword Usage</b>	Optional keyword. By default, the program uses the velocity or flow-rate from the XML Solution File.
	<b>Reactor Models</b>	<ul style="list-style-type: none"> <li>• Honeycomb Reactor</li> <li>• Perfectly Stirred Reactor (PSR)</li> <li>• Plasma Plug Flow Reactor</li> <li>• Plasma PSR</li> </ul>

Keyword	Definition			
		<ul style="list-style-type: none"><li>• Plug Flow Reactor</li><li>• Premixed Laminar Burner-stabilized Flame</li><li>• Premixed Laminar Flame-speed Calculation</li><li>• Rotating Disk CVD Reactor</li><li>• Stagnation Flow CVD Reactor</li></ul>		
USEV  XMLI	When using <a href="#">XMLI</a> , <a href="#">XMLS</a> , or <a href="#">RSTR</a> , overrides the values of velocity or flow-rate found on the XML Solution File used for restart or initialization with those specified in the user input file.			
	Keyword Usage	Optional keyword. By default, the program uses the velocity or flow-rate from the XML Solution File.		
	Reactor Models	<ul style="list-style-type: none"><li>• Cylindrical Shear Flow Reactor</li><li>• Honeycomb Reactor</li><li>• Non-reactive Gas Mixer</li><li>• Perfectly Stirred Reactor (PSR)</li><li>• Planar Shear Flow Reactor</li><li>• Plasma Plug Flow Reactor</li><li>• Plasma PSR</li><li>• Plug Flow Reactor</li><li>• Premixed Laminar Burner-stabilized Flame</li><li>• Premixed Laminar Flame-speed Calculation</li><li>• Rotating Disk CVD Reactor</li><li>• Stagnation Flow CVD Reactor</li></ul>		
US- RIN  Inlet Property	Specification of a reactor inlet stream using a user-programmed subroutine. Use of USRIN requires that a user routine SUBROUTINEUSRINLET (LIUIN, IINWRK, LRUIN, RINWRK, INAME, KNAMES, FLRT, TINL, TEIN, XIN) is written and linked to the application program. Calls to this routine will be used to obtain the corresponding flow rate ( <a href="#">FLRT</a> ), inlet temperature ( <a href="#">TINL</a> ), engine-out electron temperature ( <a href="#">TEIN</a> ), and composition ( <a href="#">REAC</a> ). See the Application Programming Interface Manual for more information on how to work with user subroutines.			
	Parameters	Optional/Reqd.	Units	Examples
	Stream	Required	--	USRIN <b>engineout 2</b>
	Reactor number (PSR clusters only)	<b>Option- al, if not defined,</b>	--	USRIN engineout <b>2</b>

Keyword	Definition			
		then re-actor #1 is assumed.		
	Keyword Usage	Optional keyword. By default, streams are defined using the <a href="#">INLET</a> and related keyword.		
	Reactor Models	<ul style="list-style-type: none"><li>• Non-reactive Gas Mixer</li><li>• Perfectly Stirred Reactor (PSR)</li><li>• Plasma PSR</li></ul>		
	Notes	<ul style="list-style-type: none"><li>• See <a href="#">User Supplemental Programming</a> of the Application Programming Interface Manual for details.</li></ul>		
UTRN  Reactor Property, User Subroutine	Use the mixture average transport properties defined in user-programmed routine CRUTRANS (for Shear Flow reactors), OPUTRANS (for Opposed-flow Flame Simulator) or PRUTRANS (for Premixed Laminar Flame or Flame-speed Calculation). See the Application Programming Interface Manual for details on how to work with user subroutines.			
	Keyword Usage	Optional keyword. By default, transport properties will be calculated based on the fundamental transport properties provided in the chemistry set.		
	Reactor Models	<ul style="list-style-type: none"><li>• Cylindrical Shear Flow Reactor</li><li>• Opposed-flow Flame Simulator</li><li>• Planar Shear Flow Reactor</li><li>• Premixed Laminar Burner-stabilized Flame</li><li>• Premixed Laminar Flame-speed Calculation</li></ul>		
UWGT  Reactor Property	Grid refinement weighting factor for the axial velocity. A value greater than 1 will increase the grid resolution outside of the reacting zone/wall region to improve the accuracy of velocity solutions near the inlet region.			
	Parameters	Optional/Reqd.	Units	Examples
	Weighting Factor	Optional	--	UWGT <b>2.0</b>
	Keyword Usage	Optional keyword. Default value is 1.		
	Reactor Models	<ul style="list-style-type: none"><li>• Rotating Disk CVD Reactor</li><li>• Stagnation Flow CVD Reactor</li></ul>		
VCOR  Reactor Property	Including this keyword causes the calculation to be run using a correction velocity to ensure mass conservation, i.e., the sum of the diffusion fluxes is zero. See <a href="#">Equation 14.11</a> of the <a href="#">Chemkin-Pro Theory Manual</a> . If <a href="#">VCOR</a> is not used, then <a href="#">TRCE</a> is in effect.			

Keyword	Definition			
	Keyword Usage	Optional keyword. By default, correction velocity is not used.		
	Reactor Models	<ul style="list-style-type: none"><li>• Cylindrical Shear Flow Reactor</li><li>• Planar Shear Flow Reactor</li><li>• Premixed Laminar Burner-stabilized Flame</li><li>• Premixed Laminar Flame-speed Calculation</li><li>• Rotating Disk CVD Reactor</li><li>• Stagnation Flow CVD Reactor</li></ul>		
VDOT	Inlet volumetric flow rate.			
Inlet Property	Parameters	Optional/Reqd.	Units	Examples
	Inlet volumetric flow rate	Required	cm <sup>3</sup> /sec	VDOT <b>100</b>
	Keyword Usage	Optional keyword. Either <b>VDOT</b> or <b>VEL</b> must be specified, unless this is a restart run. <b>PFRs and Monolith Reactors:</b> Flow specification via one of <b>VEL</b> , <b>VDOT</b> , <b>VDOTPRO SCCM SCCMPRO FLRT</b> , or <b>FPRO</b> is required.		
	Reactor Models	<ul style="list-style-type: none"><li>• Honeycomb Reactor</li><li>• Plasma Plug Flow Reactor</li><li>• Plug Flow Reactor</li></ul>		
VDOTPRO	Specifies a transient profile or function of mass flow rate vs. independent variable (time or position) for an inlet stream, in cubic centimeters per minute. The profile specified will be interpolated linearly from the <b>VDOTPRO</b> points provided.			
Inlet PropertyProfiles	Parameters	Optional/Reqd.	Units	Examples
	Inlet stream name	Optional If no stream name is given, the profile described is assumed to apply to all reactors in a cluster.	-	VDOTPRO <b>purge</b> 0.19 300
	Time (Distance for flow reactor)	Required	sec (cm	VDOTPRO purge <b>0.19</b> 300

Keyword	Definition			
			for flow reactor)	
	Equivalent volumetric flow rate	Required	cm <sup>3</sup> /min	VDOTPRO purge 0.19 <b>300</b>
	Keyword Usage	PFRs and Monolith Reactors: Flow specification via one of VEL, VDOT, VDOTPRO, SCCM, SCCMPRO, FLRT, or FPRO is required. PSRs and PaSRs: Optional keyword. If none of TAU, FLRT/FPRO, SCCM/SCCMPRO, or VDOT/VDOTPRO are specified or are nonzero, then a closed-system is assumed. FLRT/FPRO, SCCM/SCCMPRO, or VDOT/VDOTPRO is required for each INLET stream defined. Stagnation Flow CVD Reactors: FLRT/FPRO, SCCM/SCCMPRO or UINL is required for each inlet stream defined. Rotating Disk CVD Reactors: Optional keyword.		
	Reactor Models	<ul style="list-style-type: none"><li>Non-reactive Gas Mixer</li><li>Perfectly Stirred Reactor (PSR)</li><li>Plasma PSR</li><li>Plug Flow Reactor (PFR)</li><li>Plasma PFR</li><li>Honeycomb Monolith Reactor</li><li>Rotating Disk CVD Reactor</li><li>Stagnation Flow CVD Reactor</li></ul>		
VEL  Inlet Property	The gas-phase velocity at the inlet (for plug-flow reactors) or the maximum gas velocity at the inlet (for shear-flow reactors).			
	Parameters	Optional/Reqd.	Units	Examples
	Velocity	Required	cm/sec	VEL 15
	Keyword Usage	Plug Flow Reactors: Optional keyword. Either VDOT or VEL must be specified, unless this is a restart run. Shear Flow Reactors: If the problem is in cartesian coordinates, then the average velocity equals two-thirds of the maximum velocity of the parabolic velocity profile. In cylindrical coordinates, the average velocity is half of the maximum velocity. If the keyword BLTK is given, a flat velocity profile will be used, i.e., everywhere the velocity will be set equal to VEL except within a distance BLTK of the wall.		
	Reactor Models	<ul style="list-style-type: none"><li>Cylindrical Shear Flow Reactor</li><li>Honeycomb Reactor</li></ul>		



Keyword	Definition			
		<ul style="list-style-type: none"><li>Planar Shear Flow Reactor</li><li>Plasma Plug Flow Reactor</li><li>Plug Flow Reactor</li></ul>		
<b>VELPRO</b>	Flow velocity along the distance of a plug reactor.			
Reactor Property	Parameters	Optional/Reqd.	Units	Examples
	<i>Distance value</i>	Required	cm	VELPRO <b>1.0</b> 10.0
	<i>Velocity</i>	Required	cm/sec	VELPRO 1.0 <b>10.0</b>
	<b>Keyword Usage</b>	Optional keyword. By default, no profile is provided.		
	<b>Reactor Models</b>	<ul style="list-style-type: none"><li>Plug Flow Reactor</li></ul>		
<b>VF-FAC</b>	The fraction of fuel vapor to be retained in the spray parcel after vaporization. If the bulk gas and the spray parcels are traveling at different directions and speeds, a large portion of the fuel vapor could be pushed out of its originating spray parcel. This vaporization rate model parameter can be used to improve the low vaporization rate issue of fuel components with high boiling point. Reducing the value of this parameter will increase the vaporization rate. This model parameter should have a value between 0 and 1 inclusive and will be applied to all injections of the same DI engine simulation.			
Reactor Property	Parameters	Optional/Reqd.	Units	Examples
	<i>Retention fraction</i>	Optional	--	VFFAC <b>0.0</b>
	<b>Keyword Usage</b>	Optional keyword. By default, the vapor retention fraction is set to 0.01.		
	<b>Reactor Models</b>	<ul style="list-style-type: none"><li>Direct Injection Diesel Engine Simulator</li></ul>		
	<b>VH</b>	Constant volume and enthalpy constraints.		
Problem Type	<b>Keyword Usage</b>	Optional keyword. Exactly one problem-type keyword must be included.		
	<b>Reactor Models</b>	<ul style="list-style-type: none"><li>Chemical and Phase Equilibrium Calculations</li></ul>		
<b>VIS</b>	Viscosity of the inlet gas mixture.			
Inlet Property	Parameters	Optional/Reqd.	Units	Examples
	<i>Viscosity</i>	Required	g/(cm · sec)	VIS <b>0.01</b>
	<b>Keyword Usage</b>	Optional keyword. By default, the viscosity is 0, i.e., viscous drag is neglected.		
	<b>Reactor Models</b>	<ul style="list-style-type: none"><li>Honeycomb Reactor</li><li>Plasma Plug Flow Reactor</li><li>Plug Flow Reactor</li></ul>		
	<b>Notes</b>	<ul style="list-style-type: none"><li>A poise is equivalent to g/(cm · sec).</li></ul>		

Keyword	Definition			
VISC  Reactor Property	Viscosity of the mixture at 300 K. Required input for boundary layer corrections.			
	Parameters	Optional/Reqd.	Units	Examples
	Viscosity at 300 K	Required	g/(cm · sec)	VISC 2.65E-4
	Keyword Usage	Optional keyword. By default, the viscosity is not set. This keyword is required for boundary layer corrections.		
	Reactor Models	• Normal Incident Shock		
VOL  Reactor Property	The volume of the reactor. In multi-zone models, users can enter zone volume fractions rather than exact zone volumes. The software will calculate the initial cylinder volume, normalize the volume fractions, and compute the exact zone volumes at the start of simulation. VOL is used to give Zone volumes and Zone volume fractions.			
	Parameters	Optional/Reqd.	Units	Examples
	Volume	Required	cm <sup>3</sup>	VOL 1200
	Reactor number (PSR clusters only)	Optional If no number is given, the keyword is assumed to apply to all reactors in a cluster.	--	VOL 1200 <b>1</b>
	Keyword Usage	Optional keyword. By default, volume is required input for all PSRs unless		
	Reactor Models	• Closed Homogeneous Batch Reactor  • Closed Partially Stirred Reactor (PaSR)  • Closed Plasma Reactor  • Non-reactive Gas Mixer  • Partially Stirred Reactor (PaSR)  • Perfectly Stirred Reactor (PSR)  • Plasma PSR		
	VOL  Reactor Property	The fraction of the total volume inside the cylinder for each zone in a Multi-Zone HCCI Engine model.		
Parameters		Optional/Reqd.	Units	Examples

Keyword	Definition			
	Zone volume fraction	Required	--	VOL 0.15 4
	Zone number	Required	--	VOL 0.15 4
	Keyword Usage	Optional keyword.		
	Reactor Models	<ul style="list-style-type: none"><li>Multi-Zone HCCI Engine Simulator</li><li>SI Engine Zonal Simulator</li></ul>		
VOL	The initial specific volume of the gas mixture.			
Reactor Property	Parameters	Optional/Reqd.	Units	Examples
	Specific volume of the gas mixture	Required	cm <sup>3</sup> /g	VOL 1200
	Keyword Usage	Optional keyword. The user must specify two state variables and the composition to define the initial mixture.		
	Reactor Models	<ul style="list-style-type: none"><li>Chemical and Phase Equilibrium Calculations</li></ul>		
VOLC	Engine cylinder clearance volume.			
Reactor Property	Parameters	Optional/Reqd.	Units	Examples
	Engine cylinder clearance volume	Required	cm <sup>3</sup>	VOLC <b>2.0</b>
	Keyword Usage	Optional keyword. Any two of <b>VOLC</b> , <b>VOLD</b> , or <b>CMPR</b> must be specified.		
	Reactor Models	<ul style="list-style-type: none"><li>IC HCCI Engine</li><li>SI Engine Zonal Simulator</li></ul>		
VOLD	Engine displacement volume, or the volume swept by the piston during compression.			
Reactor Property	Parameters	Optional/Reqd.	Units	Examples
	Displacement volume	Required	cm <sup>3</sup>	VOLD <b>2.0</b>
	Keyword Usage	Optional keyword. Any two of <b>VOLC</b> , <b>VOLD</b> , or <b>CMPR</b> must be specified		
	Reactor Models	<ul style="list-style-type: none"><li>IC HCCI Engine</li><li>SI Engine Zonal Simulator</li></ul>		
VPARI	Initial volume of a single spray parcel.			
Reactor Property/Model	Parameters	Optional/Reqd.	Units	Examples
	initial parcel vol	Required	cm <sup>3</sup>	VPARI <b>5.0</b>
	Keyword Usage	Required keyword.		
	Reactor Models	<ul style="list-style-type: none"><li>Direct Injection Diesel Engine Simulator</li></ul>		

Keyword	Definition			
VP-MOD  Reactor Property/Model	Specify how the droplet surface temperature is determined. If VPMOD=0: uniform droplet temperature model, that is, the droplet surface temperature is the same as the droplet core temperature. If VPMOD=1: two temperature model; the droplet surface temperature is solved by the energy conservation equation at the droplet surface.			
	Parameters	Optional/Reqd.	Units	Examples
	Surface temperature model	Required	--	VPMOD <b>1</b>
	Keyword Usage	Optional keyword. Default: the uniform temperature model is used.		
	Reactor Models	• Direct Injection Diesel Engine Simulator		
VPRO  Reactor Property Profiles	Reactor volume profile specified as a function of time.			
	Parameters	Optional/Reqd.	Units	Examples
	Time value	Required	sec	VPRO <b>1.0E-4</b> 1.0
	Volume	Required	cm <sup>3</sup>	VPRO 1.0E-4 <b>1.0</b>
	Reactor number (PSR clusters only)	Optional  If no number is given, the profile described by the first two values is assumed to apply to all reactors in a cluster.	--	VPRO 1.0E-4 1.0 <b>1</b>
	Keyword Usage	For constrained-volume problems, <b>VOL</b> or <b>VPRO</b> must be specified. Otherwise, a default value of 1.0 is used for the initial reactor volume.		
	Reactor Models	• Closed Homogeneous Batch Reactor  • Closed Partially Stirred Reactor (PaSR)  • Closed Plasma Reactor  • Non-reactive Gas Mixer  • Partially Stirred Reactor (PaSR)  • Perfectly Stirred Reactor (PSR)		

Keyword	Definition			
		• Plasma PSR		
VRS  Reactor Property	Reflected shock velocity. If specified, it is used to determine the state of the gas after the shock. The reflected shock velocity is never used unless the incident shock velocity is also given.			
	Parameters	Optional/Reqd.	Units	Examples
	Reflected shock velocity	Required	cm/sec	VRS <b>100</b>
	Keyword Usage	Optional keyword. By default, no shock velocities are computed, but $U_5=0$ .		
	Reactor Models	• Normal Reflected Shock		
VS  Problem Type	Constant volume and entropy constraints.			
	Keyword Usage	Optional keyword. Exactly one problem-type keyword must be included.		
	Reactor Models	• Chemical and Phase Equilibrium Calculations		
	Notes	• <b>SV</b> keyword.is equivalent.		
VSHK  Reactor Property	Incident shock velocity.			
	Parameters	Optional/Reqd.	Units	Examples
	Velocity	Required	cm/sec	VSHK <b>3000.</b>
	Keyword Usage	This input is required for all incident shock problems, and may be used for some reflected shock problems.		
	Reactor Models	• Normal Incident Shock  • Normal Reflected Shock		
VTIM  Reactor Property	The solution will be obtained with the volume as a function of time specified through a user programmed subroutine. SUBROUTINE PSVOLT(TIME, LOUT, VOL, DVDT) must be provided to specify the volume, and linked to the application program.			
	Keyword Usage	Optional keyword. By default, volume is specified through <b>VOL</b> or <b>VPRO</b> .		
	Reactor Models	• Closed Homogeneous Batch Reactor  • Closed Plasma Reactor  • Non-reactive Gas Mixer  • Perfectly Stirred Reactor (PSR)  • Plasma PSR		
	Notes	• See also <b>VPRO</b> as an alternative way to specify volume as a function of time.		

Keyword	Definition			
		• See the Application Programming Interface Manual for more information on how to work with user subroutines.		
VU Problem Type	Constant volume and energy constraints.			
	Keyword Usage	Optional keyword. Exactly one problem-type keyword must be included.		
	Reactor Models	• Chemical and Phase Equilibrium Calculations		
	Notes	• <b>UV</b> keyword is equivalent.		
VWALL Reactor Property	Specify a constant axial slip velocity at the walls.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Axial slip velocity</i>	Required	cm/sec	VWALL <b>1.1</b>
	Keyword Usage	Optional keyword. See also <a href="#">SLIP</a> .		
	Reactor Models	• Cylindrical Shear Flow Reactor  • Planar Shear Flow Reactor		
WBFB Solver	Specifies the <i>b</i> parameter of the Wiebe function. <i>b</i> must be greater than 0 and is set to 5.0 by default.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Value of the <i>b</i> parameter</i>	Required	--	WBFB 9.0
	Keyword Usage	Optional keyword.		
	Reactor Models	• SI Engine Zonal Simulator		
WBFN Solver	Specifies the <i>n</i> parameter of the Wiebe function. <i>n</i> must be greater than 0 and is set to 2.0 by default.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Value of the <i>n</i> parameter</i>	Required	--	WBFN 4.0
	Keyword Usage	Optional keyword.		
	Reactor Models	• SI Engine Zonal Simulator		
WDIF Solver	Use windward differencing on convective terms in the equations.			
	Keyword Usage	Optional keyword. By default, windward differencing is used.		
	Reactor Models	• Diffusion or Premixed Opposed-flow Flame  • Premixed Laminar Burner-stabilized Flame  • Premixed Laminar Flame-speed Calculation		
WELL	Flag indicating that a well mixed model will be used to simulate the molecular mixing within the computational particle.			

Keyword	Definition			
Reactor Property	Keyword Usage	Optional keyword. By default, a well mixed model is assumed.		
	Reactor Models	<ul style="list-style-type: none"><li>Closed Partially Stirred Reactor (PaSR)</li><li>Partially Stirred Reactor (PaSR)</li></ul>		
WENG  Reactor Property	The reactor wall temperature will be obtained by solving energy conservation equations for the reactor wall. When WENG is used, all the external heat fluxes, i.e., heat loss to the environment and heat exchange between the reactors in a network, are applied to the wall energy equation instead of the gas phase energy equation. Also, the heat generated by surface reactions will be included in the wall energy equation. If a surface has more than one material, the wall temperature is always assigned to the first material.			
	Parameters	Optional/Reqd.	Units	Examples
	Thermal mass	Required	cal/K	WENG 0.1 500 1
	Heat transfer coefficient	Required	cal/(cm <sup>2</sup> · sec · K)	WENG 0.1 500 1
	Reactor number (PSR clusters only)	Optional  If no number is given, the keyword is assumed to apply to all reactors in a cluster.	--	WENG 0.1 500 1
	Keyword Usage	Optional keyword. By default the surface temperature is fixed. The two required numbers on the keyword line specify the thermal mass of the reactor wall and the heat transfer coefficient between the inner wall surface and the gas mixture inside the reactor. The initial wall temperature can be specified by the keyword TSRF otherwise the gas temperature will be used. For Plug Flow Reactors the <b>thermal mass parameter</b> is described in units of cal/(cm · K).		
Reactor Models	<ul style="list-style-type: none"><li>Closed Homogeneous Batch Reactor</li><li>Closed Plasma Reactor</li><li>Honeycomb Reactor</li><li>IC HCCI Engine</li></ul>			

Keyword	Definition			
		<ul style="list-style-type: none"><li>• Non-reactive Gas Mixer</li><li>• Perfectly Stirred Reactor (PSR)</li><li>• Plasma Plug Flow Reactor</li><li>• Plasma PSR</li><li>• Plug Flow Reactor</li><li>• SI Engine Zonal Simulator</li></ul>		
<b>WMIX</b>  Reactor Property	Width of the mixing region; used in defining the initial profile for the <a href="#">LINE</a> or <a href="#">PLAT</a> options.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Width of mixing region</i>	Required	cm	WMIX <b>2.0</b>
	<b>Keyword Usage</b>	Optional keyword. By default the width of the mixing region is <a href="#">XEND</a> * 0.5.		
	<b>Reactor Models</b>	<ul style="list-style-type: none"><li>• Diffusion or Premixed Opposed-flow Flame</li><li>• Premixed Laminar Burner-stabilized Flame</li><li>• Premixed Laminar Flame-speed Calculation</li><li>• Rotating Disk CVD Reactor</li><li>• Stagnation Flow CVD Reactor</li></ul>		
<b>WOSP1</b>  Reactor Property	Specify parameters of the Woschni heat transfer correlation for the compression period.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>C11 in the average gas velocity correlation.</i>	Required	--	WOSP1 2.28 0.318 0.0 1.57
	<i>C12 in the Woschni correlation.</i>	Required	cm/(sec - K)	WOSP1 2.28 0.318 0.0 1.57
	<i>C2 in the Woschni correlation.</i>	Required	--	WOSP1 2.28 0.318 0.0 1.57
	<i>Ratio of swirl velocity to mean piston speed.</i>	Required	--	WOSP1 2.28 0.318 0.0 1.57
	<b>Keyword Usage</b>	Optional keyword.		
	<b>Reactor Models</b>	<ul style="list-style-type: none"><li>• Multi-Zone HCCI Simulator</li><li>• IC HCCI Engine</li><li>• SI Engine Zonal Simulator</li></ul>		



Keyword	Definition			
<b>WOSP2</b>  Reactor Property	Specify parameters of the Woschni heat transfer correlation for the combustion period.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>C11 in the average gas velocity correlation.</i>	Required	--	WOSP2 2.28 0.318 0.0 1.57
	<i>C12 in the Woschni correlation.</i>	Required	cm/(sec - K)	WOSP2 2.28 0.318 0.0 1.57
	<i>C2 in the Woschni correlation.</i>	Required	--	WOSP2 2.28 0.318 0.0 1.57
	<i>Ratio of swirl velocity to mean piston speed.</i>	Required	--	WOSP2 2.28 0.318 0.0 1.57
	<b>Keyword Usage</b>	Optional keyword.		
	<b>Reactor Models</b>	<ul style="list-style-type: none"><li>• Multi-Zone HCCI Simulator</li><li>• IC HCCI Engine</li><li>• SI Engine Zonal Simulator</li></ul>		
<b>WOSP3</b>  Reactor Property	Specify parameters of the Woschni heat transfer correlation for the expansion period.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>C11 in the average gas velocity correlation.</i>	Required	--	WOSP3 2.28 0.318 0.0 1.57
	<i>C12 in the Woschni correlation.</i>	Required	cm/(sec - K)	WOSP3 2.28 0.318 0.0 1.57
	<i>C2 in the Woschni correlation.</i>	Required	--	WOSP3 2.28 0.318 0.0 1.57
	<i>Ratio of swirl velocity to mean piston speed.</i>	Required	--	WOSP3 2.28 0.318 0.0 1.57
	<b>Keyword Usage</b>	Optional keyword.		
	<b>Reactor Models</b>	<ul style="list-style-type: none"><li>• Multi-Zone HCCI Simulator</li><li>• IC HCCI Engine</li><li>• SI Engine Zonal Simulator</li></ul>		
<b>WPRO</b>  Reactor Property Profiles	Plasma power deposition profile specified as a function of time.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Time value</i>	Required	sec	WPRO <b>1.0E-4</b> 500
	<i>Plasma power deposition</i>	Required	watts	WPRO 1.0E-4 <b>500</b>

Keyword	Definition			
	<i>Reactor number (PSR clusters only)</i>	Optional  If no number is given, the profile described by the first two values is assumed to apply to all reactors in a cluster.	--	WPRO 1.0E-4 500 <b>1</b>
	<b>Keyword Usage</b>	Optional keyword. By default, no profile is provided.		
	<b>Reactor Models</b>	<ul style="list-style-type: none"><li>• Closed Plasma Reactor</li><li>• Plasma Plug Flow Reactor</li><li>• Plasma PSR</li></ul>		
<b>WS-RC</b>	Half-width of the Gaussian source term if the gas is being heated by an optional heat source. See <a href="#">Equation 14.12</a> of the <a href="#">Chemkin-Pro Theory Manual</a> .			
Reactor Property	Parameters	Optional/Reqd.	Units	Examples
	<i>Half-width</i>	Required	cm	WSRC <b>0.07</b>
	<b>Keyword Usage</b>	Optional keyword. By default, the half-width is 0.0. This is a required keyword when QDOT is not 0.0.		
	<b>Reactor Models</b>	<ul style="list-style-type: none"><li>• Rotating Disk CVD Reactor</li><li>• Stagnation Flow CVD Reactor</li></ul>		
<b>XBTH</b>	Specifies the bath gas composition. The [ <b>Species name</b> ] (or number as it appears in the Pre-processor output) and desired mole fraction are required parameters. If at least one species in a phase has been set with the <a href="#">XBTH</a> keyword, then all of the specified mole fractions for that phase are summed and normalized so that they add up to one. If no <a href="#">XBTH</a> parameters have been specified for any species in the phase, then mole fractions for all species in that phase are set equal to one another.			
Reactor Property	Parameters	Optional/Reqd.	Units	Examples
	<i>Species name</i>	Optional	--	XBTH <b>H2</b> 1.0
	<i>Species number value</i>	Optional	mole fractions	XBTH CH(S) <b>0.5</b>
	<b>Keyword Usage</b>	Optional keyword. By default, the table output is determined by the <a href="#">ALL</a> or <a href="#">NONE</a> keyword.		
	<b>Reactor Models</b>	<ul style="list-style-type: none"><li>• Mechanism Analyzer</li></ul>		

Keyword	Definition			
XCEN Reactor Property	Center of the mixing region; used in defining the initial profile for the <a href="#">LINE</a> or <a href="#">PLAT</a> options. Note that the fuel inlet is assumed to be located at $x=0$ .			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Center of mixing region</i>	Required	cm	XCEN <b>3.0</b>
	Keyword Usage	Optional keyword. By default the center of the mixing region is <a href="#">XEND</a> * 0.35.		
	Reactor Models	<ul style="list-style-type: none"><li>• Diffusion or Premixed Opposed-flow Flame</li><li>• Premixed Laminar Burner-stabilized Flame</li><li>• Premixed Laminar Flame-speed Calculation</li><li>• Rotating Disk CVD Reactor</li><li>• Stagnation Flow CVD Reactor</li></ul>		
XEND Reactor Property	Physical length of the computational domain, or value of $x$ at the end of the domain. Depending on the reactor, the beginning of the domain is either 0.0 or the value of <a href="#">XSTR</a> .			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Channel length</i>	Required	cm	XEND <b>25</b>
	Keyword Usage	Required keyword.		
	Reactor Models	<ul style="list-style-type: none"><li>• Cylindrical Shear Flow Reactor</li><li>• Diffusion or Premixed Opposed-flow Flame</li><li>• Honeycomb Reactor</li><li>• Planar Shear Flow Reactor</li><li>• Plasma Plug Flow Reactor</li><li>• Plug Flow Reactor</li><li>• Premixed Laminar Burner-stabilized Flame</li><li>• Premixed Laminar Flame-speed Calculation</li><li>• Rotating Disk CVD Reactor</li><li>• Stagnation Flow CVD Reactor</li></ul>		
XEST Reactor Property	For steady-state calculations, these are the estimated gas-phase mole fractions to begin the iteration. For transient problems, this keyword provides the initial values for the gas-phase mole fractions in the reactor. For example, XEST H2O 0.5 assigns an initial mole fraction of 0.5 to water vapor in the reactor.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Species name</i>	Required	--	XEST <b>H2O</b> 0.5

Keyword	Definition			
	<i>Initial fraction</i>	Required	mole fractions	XEST H2O <b>0.5</b>
	<b>Keyword Usage</b>	Transient cases: Required keyword; Steady-state cases: Optional keyword. By default, the initial or estimated gas-phase mole fractions are 0.0. For steady-state cases, if no <b>XEST</b> keywords are given, then an equilibrium calculation is performed to determine the initial estimates for the reactor composition.		
	<b>Reactor Models</b>	<ul style="list-style-type: none"><li>Perfectly Stirred Reactor (PSR)</li><li>Plasma PSR</li><li>SI Engine Zonal Simulator</li></ul>		
	<b>Notes</b>	<ul style="list-style-type: none"><li>The sum of all the estimated mole fractions should equal one. If they do not sum to one, they will be normalized and a warning message will be printed to the output file.</li></ul>		
<b>XIMN</b>  Reactor Property	Minimum mass or mole fraction value applied to intermediate species estimates, when the (default) equilibrium is used to determine product estimates. Ignored in the case that <b>INTM</b> keywords are present. In this case, the intermediate species fraction is initialized to be the average of its <b>PROD2</b> and <b>REAC</b> values; or <b>XIMN</b> , if <b>XIMN</b> is greater than this average.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Intermediate fractions</i>	Required	mole fractions	XIMN <b>1.0E-10</b>
	<b>Keyword Usage</b>	Optional keyword. By default, the intermediate fraction is set to 0.		
	<b>Reactor Models</b>	<ul style="list-style-type: none"><li>Premixed Laminar Burner-stabilized Flame</li><li>Premixed Laminar Flame-speed Calculation</li></ul>		
<b>XMLI</b>  Cluster Property	Read a solution from the XML Solution File used for initialization ( <i>XMLdata.zip</i> ), which may be a solution from any other Reactor Model (see also <b>RSTR</b> ). When initialization ( <b>XMLI</b> ) is used from an XML Solution File with spatial profiles (i.e., 1-D or channel-flow models), the initial values are actually averages of the profiles stored in the XML Solution File. The integral averages are calculated using trapezoidal integration rules.			
	<b>Keyword Usage</b>	Optional keyword. By default, the program does not look for an XML Solution File used for restart or initialization.		
	<b>Reactor Models</b>	<ul style="list-style-type: none"><li>Chemical and Phase Equilibrium Calculations</li><li>Closed Homogeneous Batch Reactor</li><li>Closed Plasma Reactor</li><li>Cylindrical Shear Flow Reactor</li></ul>		

Keyword	Definition	
		<ul style="list-style-type: none"> <li>• Diffusion or Premixed Opposed-flow Flame</li> <li>• Honeycomb Reactor</li> <li>• IC HCCI Engine</li> <li>• Mechanism Analyzer</li> <li>• Non-reactive Gas Mixer</li> <li>• Normal Incident Shock</li> <li>• Normal Reflected Shock</li> <li>• Partially Stirred Reactor (PaSR)</li> <li>• Perfectly Stirred Reactor (PSR)</li> <li>• Planar Shear Flow Reactor</li> <li>• Plasma Plug Flow Reactor</li> <li>• Plasma PSR</li> <li>• Plug Flow Reactor</li> <li>• Premixed Laminar Burner-stabilized Flame</li> <li>• Premixed Laminar Flame-speed Calculation</li> <li>• Rotating Disk CVD Reactor</li> <li>• SI Engine Zonal Simulator</li> <li>• Stagnation Flow CVD Reactor</li> </ul>
	<b>Notes</b>	<ul style="list-style-type: none"> <li>• For shear-layer flow solutions, we use the value integrated over the height (or radius) and divided by the cross-sectional area for the specified axial-distance location.</li> <li>• For Opposed-flow Flames and CVD Reactors, we use the value integrated over the spatial domain, divided by the total axial distance.</li> </ul>
<b>XMLS</b>  Cluster Property	Use a previously stored XML Solution File or the XML Solution File from an upstream reactor to initialize the inlet conditions of this inlet.	
	<b>Keyword Usage</b>	Optional keyword. By default, the program does not look for an XML Solution File used restart or initialization.
	<b>Reactor Models</b>	<ul style="list-style-type: none"> <li>• Cylindrical Shear Flow Reactor</li> <li>• Diffusion or Premixed Opposed-flow Flame</li> </ul>

Keyword	Definition			
		<ul style="list-style-type: none"><li>• Honeycomb Reactor</li><li>• Non-reactive Gas Mixer</li><li>• Partially Stirred Reactor (PaSR)</li><li>• Perfectly Stirred Reactor (PSR)</li><li>• Planar Shear Flow Reactor</li><li>• Plasma Plug Flow Reactor</li><li>• Plasma PSR</li><li>• Plug Flow Reactor</li><li>• Premixed Laminar Burner-stabilized Flame</li><li>• Premixed Laminar Flame-speed Calculation</li><li>• Rotating Disk CVD Reactor</li><li>• Stagnation Flow CVD Reactor</li></ul>		
<b>XRES</b> Restart	Force the starting distance for the new solution to be this value and ignore the value of distance from the XML Solution File used for restart or initialization.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Initial distance</i>	Required	cm	XRES <b>10</b>
	<b>Keyword Usage</b>	Optional keyword. By default, the value of the XML Solution File is used during a continuation or restart run.		
	<b>Reactor Models</b>	<ul style="list-style-type: none"><li>• Honeycomb Reactor</li><li>• Plasma Plug Flow Reactor</li><li>• Plug Flow Reactor</li></ul>		
<b>XRST</b> Restart	This keyword is valid when using <a href="#">RSTR</a> option. In this case, select the values to use in restart as those corresponding to the distance that is closest to (greater than or equal to) the specified distance.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Distance</i>	Required	cm	XRST <b>5.0</b>
	<b>Keyword Usage</b>	Optional keyword. By default, the point where the previous solution ended is used.		
	<b>Reactor Models</b>	<ul style="list-style-type: none"><li>• Cylindrical Shear Flow Reactor</li><li>• Planar Shear Flow Reactor</li></ul>		
<b>XSDF</b>	Default value for a momentum-transfer cross-section between electrons and each species. This value is used for all species not specified with the <a href="#">XSEK</a> keyword.			

Keyword	Definition			
Reactor Property	Parameters	Optional/Reqd.	Units	Examples
	Momentum-transfer cross-section	Required	cm <sup>2</sup>	XSDF <b>1.0E-16</b>
	Keyword Usage	Optional keyword. By default, the cross-section value is 0. In a plasma problem the user must either specify <a href="#">XSDF</a> or include an <a href="#">XSEK</a> keyword for all species except electrons.		
	Reactor Models	<ul style="list-style-type: none"><li>• Closed Plasma Reactor</li><li>• Plasma Plug Flow Reactor</li><li>• Plasma PSR</li></ul>		
XSEK  Reactor Property	Momentum-transfer collision cross-section between electrons and a specified species. For example, "XSEK AR 1.0E-16" would indicate a momentum-transfer cross-section of 10 <sup>-16</sup> cm <sup>2</sup> between electrons and argon atoms. For any species not specified by the <a href="#">XSEK</a> keyword, a user-specified default value will be used.			
	Parameters	Optional/Reqd.	Units	Examples
	Species	Required	--	XSEK <b>AR</b> 1.0E-16
	Momentum-transfer cross-section	Required	cm <sup>2</sup>	XSEK AR <b>1.0E-16</b>
	Keyword Usage	Optional keyword. By default, the cross-section value is 0. In a plasma problem the value for every species is specified by the <a href="#">XSDF</a> keyword.		
	Reactor Models	<ul style="list-style-type: none"><li>• Closed Plasma Reactor</li><li>• Plasma Plug Flow Reactor</li><li>• Plasma PSR</li></ul>		
XSRC  Reactor Property	Height above the disk which is the center of a Gaussian-shaped power source. See <a href="#">Equation 14.12</a> of the <a href="#">Chemkin-Pro Theory Manual</a> .			
	Parameters	Optional/Reqd.	Units	Examples
	Height	Required	cm	XSRC <b>0.6</b>
	Keyword Usage	Optional keyword. By default, the height is 0.0.		
	Reactor Models	<ul style="list-style-type: none"><li>• Rotating Disk CVD Reactor</li><li>• Stagnation Flow CVD Reactor</li></ul>		
XSTR  Reactor Property	The beginning of the computational domain. For burner-stabilized flames, this is the burner location.			
	Parameters	Optional/Reqd.	Units	Examples
	Inlet axial position	Required	cm	XSTR <b>1.5</b>
	Keyword Usage	Optional keyword. By default, the starting or inlet axial position is 0.		

Keyword	Definition			
	<b>Reactor Models</b>	<ul style="list-style-type: none"><li>• Honeycomb Reactor</li><li>• Plasma Plug Flow Reactor</li><li>• Plug Flow Reactor</li><li>• Premixed Laminar Burner-stabilized Flame</li><li>• Premixed Laminar Flame-speed Calculation</li><li>• Rotating Disk CVD Reactor</li><li>• Stagnation Flow CVD Reactor</li></ul>		
<b>XT-MP</b>  Reactor Property	If <b>TSRF</b> is used to specify the surface temperature, the application will set the surface temperature to <b>TINL</b> at $x=0$ and smoothly ramp the temperature up to <b>TSRF</b> at a distance of <b>XTMP</b> .			
	Parameters	Optional/Reqd.	Units	Examples
	<i>distance between TINL point and TSRF point</i>	Required	cm	XTMP <b>0.25</b>
	<b>Keyword Usage</b>	Optional keyword. By default, the distance is set to 0.5.		
	<b>Reactor Models</b>	<ul style="list-style-type: none"><li>• Cylindrical Shear Flow Reactor</li><li>• Planar Shear Flow Reactor</li></ul>		
<b>ZONEAVG</b>  Output	Flag to store only the zone-average solution data in the Multi-Zone HCCI Engine Simulator.			
	<b>Keyword Usage</b>	Optional keyword. By default, all solution data is stored in the Multi-Zone HCCI Engine Simulator output.		
	<b>Reactor Models</b>	<ul style="list-style-type: none"><li>• Multi-Zone HCCI Engine Simulator</li><li>• SI Engine Zonal Simulator</li></ul>		



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